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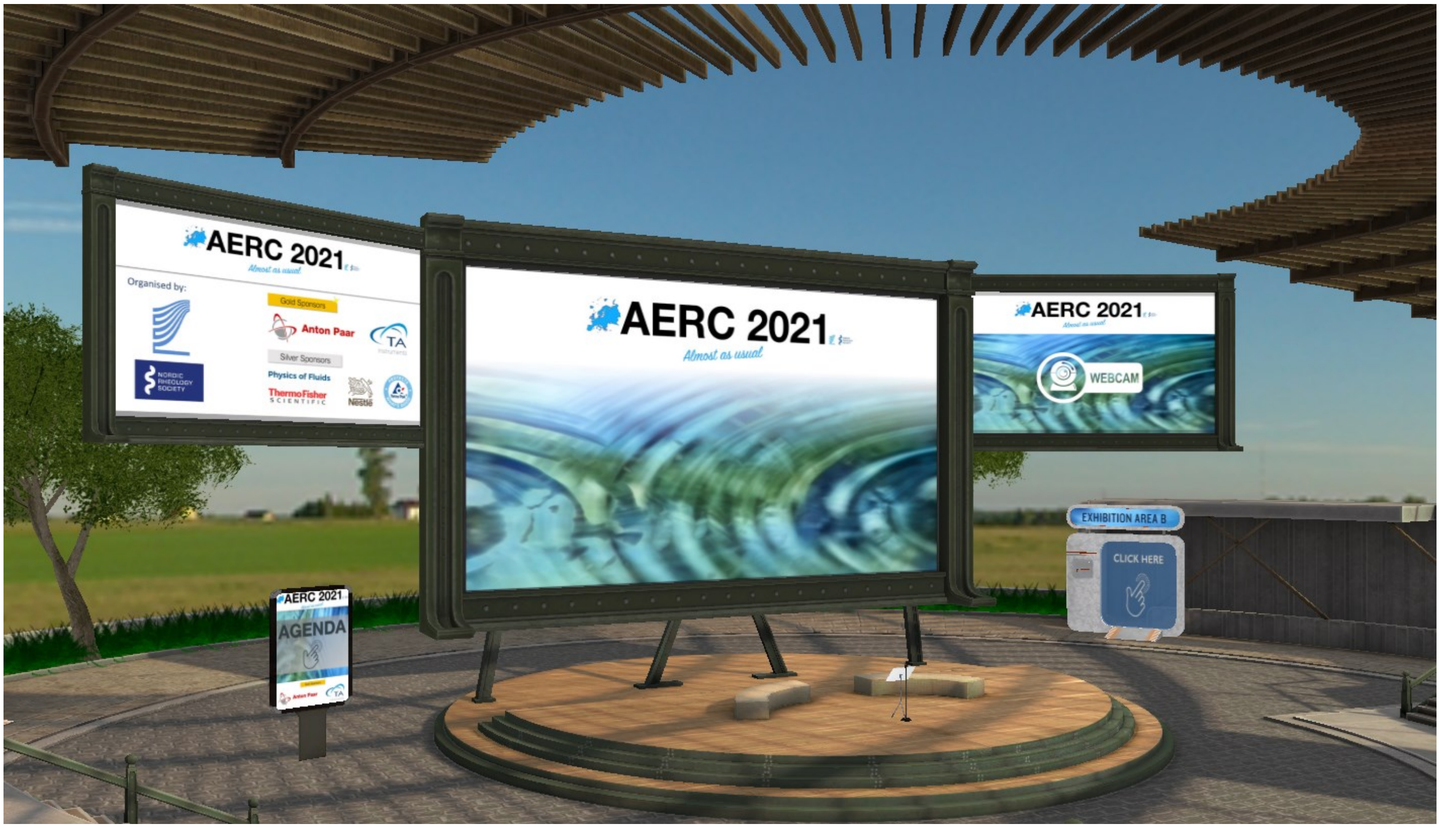
14th Annual European Rheology Conference

Cyberspace

April 13-15, 2021

BOOK OF ABSTRACTS



Annual European Rheology Conference (14 ; 2021 ; Cyberspace)
Book of abstracts / 14th Annual European Rheology Conference, 13th-15th April 2021, Cyberspace ; [editors Maria Teresa Cidade, Alexandra Aulova, Albert Co] : ESR – European Society of Rheology and Nordic Rheology Society 2021

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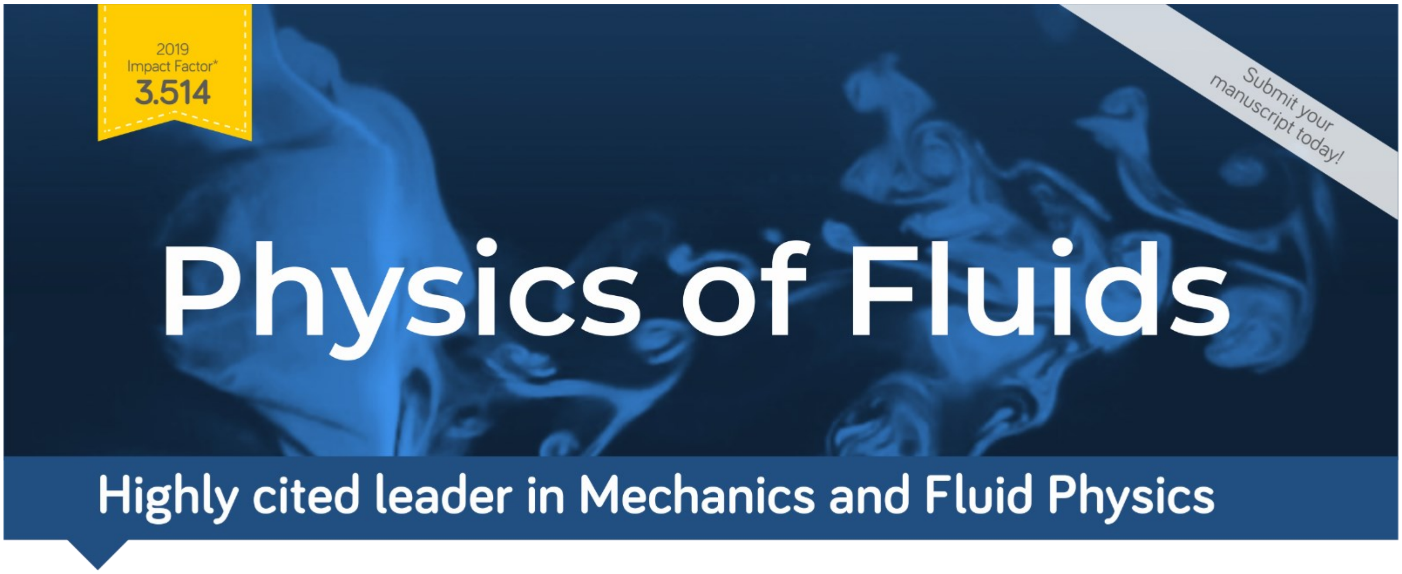

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Welcome to AERC 2021

NORDIC RHEOLOGY SOCIETY

Almost as usual

We welcome you to the 14th Annual European Rheology Conference (AERC), April 13-15, 2021 in …*Cyberspace*. The meeting is addressed to rheologists of all scientific backgrounds, from academia to industry and government research centres, aiming at sharing ideas in a friendly, informal atmosphere.

This year's AERC marks a memorable occasion for two reasons. Firstly, due to the ongoing coronavirus pandemic, for the first time the AERC is held entirely online in a virtual world with user-controlled interacting avatars. The virtual world platform was supplied by Virtway (Oviedo, Spain), styled on the 29th Nordic Rheology Conference, August 25-26, 2020, and designed and administered by Omniprex (Barcelona, Spain). Secondly, for the first time in the history of the AERC, the conference is organized by a pan-European organizing committee of volunteers. The initiative was backed by the European Society of Rheology (ESR) and the Nordic Rheology Society (NRS). The conference chairs are Roland Kádár (Chalmers, Sweden) and Mats Stading (RISE, Sweden), and Olli-Ville Laukkanen (RWTH Aachen, Germany) is the committee secretary. The other members of the organizing committee are (in alphabetical order): Johanna Andersson (RISE, Sweden), Alexandra Aulova (University of Ljubljana, Slovenia), Maria Teresa Cidade (Universidade Nova de Lisboa, Portugal), Christian Clasen (KU Leuven, Belgium), Jan Engmann (Nestlé, Switzerland), Peter Fischer (ETH Zürich, Switzerland), Anke Lindner (ESPCI Paris, France), Mario Minale (University of Campania "Luigi Vanvitelli", Italy), George Petekidis (FORTH and University of Crete, Greece) and Daphne Weihs (Technion, Israel).

The conference program features 12 sessions spanning diverse, highly relevant rheological topics, with 3 plenary presentations, 306 oral presentations and 56 poster presentations. Overall, there are over 450 participants, with authors coming from 39 countries with about 15% of the contributions from outside Europe. A short rheology course is given before the conference on 'Colloidal suspensions with focus on colloidal gels and applications' by. Norman J Wagner (University of Delaware, USA) and George Petekidis (FORTH / University of Crete, Greece). The event enjoyed the support of 7 sponsors, with two additional special event sponsors, and 6 exhibitors, which are listed in this book.

We wish to express special thanks to the ESR and NRC for making the event possible, the organizing committee, session chairpersons and instructors of the short rheology course for their hard work and cooperation, and Albert Co (University of Maine, USE) for his administering of the abstract submission website. Everyone's hard work was essential for the conference organization and it has been our privilege to serve the European rheological community.

AERC 2021 Conference Chairs,
Roland Kádár and Mats Stading

Organizers

Conference chair: Roland Kádár, Chalmers University of Technology, Sweden

Conference co-chair: Mats Stading, RISE Research Institutes of Sweden, Sweden

Conference secretary: Olli-Ville Laukkanen, RWTH Aachen University, Germany

Registration: Peter Fischer, ETH Zürich, Switzerland

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Book of abstracts: Maria Teresa Cidade, Universidade NOVA de Lisboa, Portugal

Rheology Course: George Petekidis, University of Crete IESL-FORTH, Greece

Organization committee delegates (in alphabetical order)

Johanna Andersson, RISE Research Institutes of Sweden

Christian Clasen, KU Leuven, Belgium

Roos de Smet, KU Leuven, Belgium

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Anke Lindner, ESPCI and Paris University, France

Mario Minale, Università della Campania "Luigi Vanvitelli", Italy

Daphne Weihs, Technion-Israel Institute of Technology, Israel

Symposia Organizers/Chairpersons

Session	*Keywords*	*Chairpersons*
Colloids and suspensions	Dispersions, colloids, cementitious fluids	George Petekides, Valeria Garbin
Interfacial rheology, emulsions and foams	Rheology at interfaces, emulsification, foaming	Anniina Salonen, Nikolai Denkov
Polymer melts and composites	Processing, blends, copolymers, elastomers	Maria Teresa Cidade, Juan de Vicente
Flow instabilities	Shear banding, processing effects, extrusion defects	Sandra Lerouge, Mahdi Davoodi
Modelling and simulations	Theoretical focus: computational non-Newtonian fluid mechanics, constitutive equations	Natalie Germann, Daniel Read
Complex flows	Flow focus: Multiphase flow, geological flows, complex geometries, drilling operations, processing equipment	Rossana Pasquino, Francisco Galindo Rosales
Multiphase and other complex fluids	Material focus: multiphase fluids, liquid crystals, drilling fluids, electrolytes, composites	Mario Minale, Dganit Danino
Food and bio-rheology	Food systems, biopolymers, cosmetics, pharma, cellulose fibres, pulp	Jan Engmann, Clément de Loubens
Living and self-assembling systems	Cells, tissue, swimmers, active systems, biofluid rheology	Daphne Weihs, Jan Vermant
Powder rheology, granular flows and rheology of solids	Glasses, jamming, granular media, powder flow, highly filled systems	Alexandra Aulova, Stefan Gstöhl
Experimental methods and rheometry	New or improved techniques, instruments, combined techniques	Christian Clasen, Mariana Rodríguez Hakim
Micro and nano fluidics, and microrheology	Micro channel flow, micro probes, nano particles	Anke Lindner, Laura Casanellas

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The contents of this publication were generated from the database of AERC abstract submission web site at https://www.rheology.org/aercabst/.
Online version is available at https://www.rheology.org/aerc2021/.

Tuesday Afternoon

Symposium CS

Colloids and suspensions

Organizers: George Petekides and Valeria Garbin

Tuesday 13:20 Virtual / Track 1 CS1

Normal stress waves in shear thickening suspensions

Anaïs Gauthier, Mickaël Pruvost, and Annie Colin
Chemistry Biology Innovation, ESPCI Paris-PSL, Paris 75005, France

Shear thickening (the increase of the viscosity of a fluid with the stress or the shear rate) is typical of well stabilized concentrated suspensions of hard particles. It is often associated with complex spatio-temporal fluctuations, which are not understood yet. Here, we characterize the flow of an emblematic shear thickening liquid (a cornstarch suspension) using an in-house pressure sensor array. The sensor is used in a parallel plate geometry, where it replaces the bottom plate of the rheometer. It gives access to a map of the local normal stresses within the fluid, by measuring the *zz* component of the stress on 25 regularly spaced points (of surface 4x4 mm^2 each). Intriguingly, in cornstarch suspensions, the sensors evidence a single and stable normal stress wave, rotating in the same direction as the surrounding fluid - but not at the same speed. This stress wave appears only in the discontinuous shear thickening regime, and its amplitude increases with the applied stress. We characterize this heterogeneity, and show how its shape and its relative velocity vary with the solid fraction of the suspension and the gap height. We finally discuss its origin, and compare it to the measurements obtained in different suspensions.

Tuesday 13:40 Virtual / Track 1 CS2

Microstructure and Rheology of Shear-Thickening Colloidal Suspensions with Varying Interparticle Friction: Comparison of Experiment with Theory and Simulation Models

Yu-Fan Lee[1], Yimin Luo[2], Tianyi Bai[1], Carlos A. Velez[3], Scott C. Brown[3], and Norman J. Wagner[1]
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The shear thickening of dense colloidal suspensions is an active area of research aimed to understand the highly nonlinear increase of viscosity under various processing conditions. Efforts in theoretical models and simulations seek to examine the fundamental physics for strong to discontinuous shear thickening, which is thought to be controlled by nanometric tangential inter-particle forces, such as enhanced lubrication hydrodynamics [1,2] or frictional contact forces [3-5], whereas experimental tests of these latest theories are lacking especially in microstructure at particle level. In this work, we present rheological and microstructural comparisons between two model suspensions, bare and coated model spheres with known friction level, and two competing models, friction contact model [3] and enhanced lubrication hydrodynamics [1]. It is found that opposite trend in first normal stress differences for two model suspensions can distinguish between these micromechanical mechanisms for shear thickening, and this difference is reflected in shear-induced microstructures measured via small angle neutron scattering. Statistical comparison of experiments with simulations indicates that better resolution of microstructures in simulation models are required to be validated by the experimental data presented. In general, investigation of rheology and microstructure provide quantitative information valuable to understand the mechanistic role of lubrication hydrodynamics and frictional contact in shear thickening.

[1] M. Wang, S. Jamali, and J. F. Brady, Journal of Rheology 64, 379 (2020). [2] S. Jamali and J. F. Brady, Phys. Rev. Lett. 123, 138002 (2019). [3] R. Mari, R. Seto, J. F. Morris, and M. M. Denn, Journal of Rheology 58, 1693 (2014). [4] J. F. Morris, Annual Review of Fluid Mechanics 52, null (2020). [5] R. Seto, R. Mari, J. F. Morris, and M. M. Denn, Phys Rev Lett 111, 218301 (2013).

Tuesday 14:40 Virtual / Track 1 CS3

Simulations of highly concentrated frictional suspensions with a Sommerfeld-number-dependent friction coefficient

Jose A. Ruiz-Lopez[1], Sagaya P. Savarimuthu[1], Adolfo Vazquez-Quesada[2], and Marco Ellero[1]
[1]Computational Mathematics - CFD Modelling and Simulation, BCAM - Basque Center for Applied Mathematics, Bilbao, Spain; [2]Autonomous University of Madrid, Madrid, Madrid 28049, Spain

Highly-concentrated suspensions of particles with repulsive interactions typically exhibit a shear-thickening behavior which depends on their concentration. The suspension viscosity increases and, eventually, at high concentrations, the viscosity diverges and the sample jams. This behavior has been recently explained in terms of "frictional contacts" between particles in experiments and simulations [1]. Frictional contacts provide an effective geometrical constraint for the movement of the particles, blocking the system and increasing the viscosity. In a friction-

dominated regime, the contact friction coefficient determines the rheology of the suspension. The higher the friction coefficient, the smaller the critical "jamming" concentration [1]. In spite of the progresses made in the modelling and understanding of frictional suspensions, simulations do usually employ a constant friction coefficient between particles. With the exception of [2-3], where a variable load-dependent friction coefficient was used, not many works have focused on this aspect. From experiments and simulations in tribology, it has been often reported that the friction coefficient between two surfaces depends on the normal force acting on the surfaces and the relative tangential sliding velocity. Particle-level simulations of hard spheres using short-range lubrication and frictional forces based on our recent model [6], are carried out by adopting an additional variable friction coefficient as function of the so-called local Sommerfeld number (the ratio between the inter-particle tangential velocity and the normal force). Results show that the bulk rheological properties of the suspensions are highly dependent on the tribological model used for interparticle friction, the elastic properties of the particles and their concentration.

[1] Mari et al. J. Rheol., 58, 1693-1724 (2014) [2] Lobry et al. , J. Fluid Mech., 860, 682-710 (2019) [3] More and Ardekani, J. Rheol. 64, 67 (2020) [4] Prasanna Kumar et al., J. Comp. Phys., 427, 110001 (2021)

Tuesday 15:00 Virtual / Track 1 CS5

Rheological behavior of shear-thickening nanofluids: effect of nanoparticle size and surface chemistry

Parvin Alaee, Milad Kamkar, and Mohammad Arjmand
University of British Columbia, Kelowna, BC, Canada

Polyethylene Glycol (PEG)/silica nanoparticles (NPs) suspensions have been widely used as shear-thickening fluids for advanced applications such as bullet-proof vests. In this study, the effects of different fumed silica nanoparticles (NPs) varying in surface chemistry and particle size on linear and nonlinear rheological behavior of fumed silica NPs- PEG suspensions were investigated. The silica-PEG samples with different amounts of silica NPs were prepared by a mechanical mixer. The shear thickening behavior of silica-PEG samples was studied using a rotational rheometer in a steady state flow mode. Silica 200 (hydrophilic with average particle size (APS) of 12 nm)-PEG and silica 816 (slightly hydrophobic with APS of 12 nm)-PEG samples showed a strong shear thickening behavior at concentrations above 20 wt. %. Whereas silica 300 (hydrophilic with APS of 7 nm)-PEG suspensions follow a different scenario and their flow behavior features a shear thinning behavior at all concentrations. Critical shear rate (onset of shear thickening behavior) for 20 wt. % silica 200-PEG and 20 wt. % silica 816-PEG was determined to be 79.6 and 231 s-1, respectively indicating the effect of surface chemistry on shear thickening behavior. The extent of shear thickening behavior of silica 200 incorporated samples was also extremely higher than silica 816 incorporated samples. In the last step of this work, we scrutinized the effect of temperature on shear thickening behavior of silica 200-PEG and silica 816-PEG. Results showed dramatic sensitivity of shear thickening response to the temperature.

Symposium PM

Polymer melts and composites

Organizers: Maria Teresa Cidade and Juan de Vicente

Tuesday 13:20 Virtual / Track 2 PM1

Rheological and adhesion properties of UV light photoactivated castor oil-based polyurethane adhesives

Antonio M. Borrero-López[1], David Guzmán[2], José A. González-Delgado[2], Concepción Valencia[1], Uwe Pischel[2], and José M. Franco[1]
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This study deals with the formulation and rheological characterization of UV-curable polyurethane bio-based adhesives, comprising castor oil as polyol source, methylene diphenyl diisocyanate (MDI) as crosslinker and a diamine such as cadaverine once protected with 4,5-dimethoxy-2-nitrobenzyl carbonochloridate (nVoc), a well-known photolabile protecting reagent. The UV-light irradiation triggers the photorelease of those protected diamine molecules, which tend to react with MDI much faster than castor oil hydroxyl groups, to form polyureas, thus initiating and accelerating the curing process. A significant increase of the SAOS viscoelastic functions of more than two decades was eventually found while irradiating for a 6-h period. Moreover, UV-light also induces the adhesive to pass from liquid-like to a strong gel-like state, exhibiting a difference of one order of magnitude between the storage and loss moduli at 6 h. This photoactivated change in rheological response is also associated with a noticeable increase in the adhesion strength. Thus, the performance of non-irradiated samples on PET specimens after 24 h (1.5 MPa shear strength) is easily achieved by the same adhesive but irradiated with UV-light after 2-3 h and 3-fold increased after 4 h. Furthermore, it has also been demonstrated that the higher the intensity of the UV-light, the faster and stronger the chemical crosslinking and H-bonding interactions formed, due to the release of more cadaverine within the mixture, finally raising adhesive strength values. Nonetheless, the use of cadaverine without nVoc protection does not lead to the formation of potential adhesives, suggesting the stepwise liberation of the diamines together with the occurrence of the reaction between MDI and castor oil to form urethane linkages are the reason for those remarkable outcomes observed.

Acknowledgements. This work is part of a research project (UHU-1252599) sponsored by the FEDER-Junta de Andalucía 2014-2020 Operational Programme.

Tuesday 13:40 Virtual / Track 2 PM2

Nonlinear Shear Rheometry of Unentangled Polystyrene Melts

Salvatore Costanzo[1], Katerina Peponaki[2], Stelios Alexandris[2], Daniele Parisi[2], Nino Grizzuti[1], and Dimitris Vlassopoulos[2]
[1]DICMaPI, Università degli Studi di Napoli Federico II, Napoli, Italy; [2]FORTH, Heraklion, Greece

Decoding the dynamics of polymers in fast flows is an outstanding challenge. On the experimental side, fast flows are prone to flow instabilities and require suitable setups to collect reliable data over a wide range of shear rates. On the theoretical side, recent progress reveals the importance of phenomena such as monomeric friction reduction and finite chain extensibility. In the past, many research efforts were devoted to exploring nonlinear dynamics of entangled polymers. Reliable elongational data at high Weissenberg number were obtained with the filament stretching rheometer. On the other hand, the cone-partitioned plate rheometry allowed to circumvent the complication of edge fracture and to perform shear start-up experiments at high rates. At the same time, tube-based models were implemented for successfully describing the dynamics of polymer melts and concentrated solutions. With this background, addressing the nonlinear rheology of unentangled polymers has emerged as a prime research topic. Unentangled polymers are thought to be relatively easy to predict, as orientation and stretch occur simultaneously. However, the available experimental data are scarce because of the associated measurement issues. For example, in shear flow, the available range of rates for nonlinear tests, between the inverse of the Rouse time and the shear rate where glassy modes come into play provoking transducer resonance, is quite narrow. Secondly, at high shear rates, instabilities such as edge fracture occur. Matsumyia et al. measured the nonlinear elongational rheology of unentangled melts. In this work, we present careful data on nonlinear start-up shear experiments on well-characterized unentangled polystyrene melts. The transient response, shear thinning behaviour and the validity of the Cox-Merz rule are discussed. Where possible, comparison with existing data and available modeling and simulation results are made.

Matsumiya et al. Macromol., 2018, 51, 9710-9729; Ianniruberto et al., Macromol., 2020, 53, 4, 1338-1345

Tuesday 14:40 Virtual / Track 2 PM3

A comparison of two rheological techniques for determining the longest relaxation time of amorphous polymers

Matthew T. Elsmore and Davide De Focatiis
Faculty of Engineering, University of Nottingham, Nottingham NG72RD, United Kingdom

A number of polymer applications require an orientation-free structure to be achieved, particularly for optical components or in cases where the absence of residual stress is necessary. The terminal relaxation time for a polymer network represents the timescale associated with the longest network chain 'forgetting' its initial orientation, and is considered an essential parameter for determining minimum melt processing cycle times for amorphous materials in such circumstances. The terminal relaxation time is conventionally measured using frequency-shifted mastercurves from dynamic rheometry, estimated from the inverse of the lowest frequency at which the elastic and viscous shear moduli intersect. For some amorphous systems, including those with low molecular weight, a dynamic modulus crossover is not observed and hence, an alternative experimental approach is required. Rotational shear rheometry is used to provide measurements of flow viscosity as a function of shear rate for a given melt temperature. Through time-temperature superposition shifting of viscosity and shear rate values to produce a viscosity mastercurve, flow performance may be predicted for any given processing temperature. The widely accepted Carreau, for monodisperse, and Cross, for polydisperse, viscosity models both include relaxation time terms which are associated with the longest relaxation time. This work looks to compare these different methods of obtaining a terminal relaxation time and the associated shift factors, from oscillatory and rotational rheometry, for a series of monodisperse and polydisperse polystyrenes. Relaxation times for a bimodal low molecular weight polystyrene, a butyl methacrylate and a novel sustainable copolymer from pyrolysed biomass, for which the conventional oscillatory method cannot be used, are then determined based on rotational rheological measurements.

Tuesday 15:00 Virtual / Track 2 PM4

Flow-induced crystallization of polylactides in capillary flow

Ziyue Zhang and Savvas G. Hatzikiriakos
Department of Chemical and Biological Engineering, University of British Columbia, Vancouver, BC V6T1Z3, Canada

Polylactide (PLA) is a biodegradable thermoplastic polyester produced from renewable biomass sources. The low crystallinity and the low associated crystallization kinetics have a negative impact on its mechanical and barrier properties. In this paper, the effect of flow-induced crystallization (FIC) of two PLA with different microstructures (different PLLA content) was studied using simple shear, uniaxial extension and capillary flow experiments. Generally, in simple shear and capillary flow, increase in shear rate and decrease in temperature was found to enhance the crystallization kinetics particularly for Weissenberg numbers (based on the reptation relaxation time, Wi) greater than 1. On the other hand, in uniaxial extensional flow, once a critical Hencky strain is achieved, crystallization starts independent of strain rate and temperature. The amount of mechanical work per unit volume imposed/dissipated onto the polymers during flow to initialize crystallization was calculated in capillary flow. The work was found to be independent of temperature and degree of molecular chain stretch (Wi) as Wi becomes greater than 1. Lastly, the PLA sample with higher content of PLLA showed slightly higher zero-shear viscosity and a smaller thermodynamic barrier for crystallization to occur.

Symposium IR

Interfacial rheology, emulsions and foams

Organizers: Anniina Salonen and Nikolai Denkov

Tuesday 13:20 Virtual / Track 3 IR1

The effect of surfactants on jet break-up in drop-on-demand inkjet printing

Evangelia Antonopoulou[1], Oliver G. Harlen[2], and Mark A. Walkley[3]

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The rapid development of new applications for inkjet printing and increasing complexity of the inks has created a demand for in-silico optimisation of the ink jetting performance. Surfactants are often added to aqueous inks to modify the surface tension. However, the rapid expansion of the free surface during the fast jetting process means local areas of the surface will be depleted of surfactants leading to surface tension gradients. We present numerical simulations of inkjet break-up and drop formation in the presence of surfactants investigating both the surfactant transport on the interface and the influence of Marangoni forces on break-up dynamics. In particular, the initial phase of a "pull-push-pull" drive waveform leads to a concentration of surfactants at the front of the main drop with the trailing ligament being almost surfactant free. The resulting Marangoni stresses act to delay and can even prevent the break-off of the main drop from the ligament. The presence of surfactants also reduces the mobility of the surface of the droplet, modifying the internal flow within the droplet and enhancing the viscous dissipation. We will also discuss the impact of surfactants on the frequency and decay of droplet oscillations.

Tuesday 13:40 Virtual / Track 3 IR2

Nonlinear surface rheology and microstructure imaging of protein – lipid mixtures

Jack Yang, Leonie Waardenburg, Claire C. Berton-Carabin, Constantinos V. Nikiforidis, Erik Van Der Linden, and Leonard M. Sagis

Wageningen University and Research, Wageningen, The Netherlands

Plant seed store oils in oleosomes (also known as oil bodies or lipid droplets), which are storage organelles with a triacylglycerol (TAG) core surrounded by a phospholipid monolayer and proteins. Due to their membrane, oleosomes are surface-active and have a potential as an emulsifier. The influence of the surface-active oleosomes on protein stabilised interfaces has not yet been studied. Therefore, we mixed rapeseed oleosomes with a well-characterised model protein, whey protein isolate (WPI), to study their air-water interfacial properties. We discovered that oleosomes rupture after adsorption at the interface, and AFM images of the interfacial microstructure showed TAG/phospholipid-rich regions and membrane fragments, resulting in a weak and mobile interfacial layer. Mixing oleosomes with WPI resulted in an interface with TAG/phospholipid-rich regions surrounded by WPI clusters. To understand the contribution of the different components on the interfacial properties, defatted oleosomes and rapeseed phospholipids (lecithin) were mixed with WPI, which also resulted in a protein-lipid mixed interfacial film. At small deformations, the lipids dominated the rheological properties, thus forming weak interfaces with limited in-plane interactions between interfacial stabilisers. When increasing the deformation amplitude into the nonlinear viscoelastic (NLVE) regime, the lipids were pushed out, and the WPI started interacting. As a result, the WPI at the mixed interface started dominating the rheological properties, showing the behaviour of a stiff and viscoelastic solid-like layer. Mixing WPI and rapeseed lipids resulted in mixed interfaces, as demonstrated by microstructure imaging and interfacial rheology, which is an important finding for the utilisation of oleosomes as an emulsifier.

Tuesday 14:40 Virtual / Track 3 IR3

The Rheology and Microstructure of Polyacrylates and Polymethylacrylates at the Air/Water Interface

Daniel Ashkenazi[1], Stelios Alexandris[2], Jan Vermant[3], Dimitris Vlassopoulos[2], and Moshe Gottlieb[1]

[1]Chemical Engineering, Ben Gurion University, Beer Sheva, Israel; [2]FORTH, Heraklion, Greece; [3]Department of Materials, ETH, Zurich, Switzerland

Polymer laden fluid interfaces play a crucial role in many biological and industrial process. Exploration of the still poorly understood interplay between polymer molecular characteristics, polymer organization at the interface, and their effect on the mechanical properties of the interface is a prerequisite for a proper design for multitude of interface dominated processes. In this contribution we investigate how the chemical structure of a series of acrylic polymers which determine chain flexibility (Tg) and anchoring to the water subphase (acrylates vs. methylacrylates) affect the evolution of the interfacial phases and the formation of an elastic interface at the air/water interface. A combination of classical rectangular Langmuir-Pockels trough, Brewster's angle microscopy for morphology and layer thickness determination, and different shear interfacial rheometers have been employed. We find that the gradual change from the highly flexible polymer poly(n butyl acrylate) to the glassy polymer poly(tert-butyl methacrylate), is accompanied by a gradual transition in the microstructure from completely liquid interface composed of discrete islets of polymer to a uniform elastic sheet. The changes in the microstructure are manifested by large variations in the interfacial rheological properties of the polymeric interface.

Tuesday 15:00 Virtual / Track 3 IR4

Effect of polysaccharides on interfacial properties of vegetable proteins at O/W interfaces

Olga Mileti, Noemi Baldino, Roberta E. Faragò, Francesca R. Lupi, and Domenico Gabriele
Department D.I.M.E.S., University of Calabria, Rende, Cs 87036, Italy

Food products are often multiphasic systems and proteins are frequently used as stabilizing agents and texture modifiers. Proteins, due to their amphiphilic structure, have good interfacial activity and are able to form viscoelastic interfacial layers. Vegetable proteins (VPs) are today extensively used as an alternative to animal protein, due to their beneficial health effects, also as well as being a suitable alternative for those suffering from allergies, intolerances or who for ethical reasons doesn't consume products of animal origin. The effect of the presence of polysaccharide species on the behaviour exhibited by VPs at the interface is poorly studied. This work aims to study the effect of some polysaccharides on the interfacial rheological behaviour of VPs at the interface O/W, using both commercial and purified sunflower oil. Hemp and brown rice proteins have been chosen to the investigation and the interfaces were investigated in dilatational kinematic, by using pendant drop tensiometer. Static and dynamic measurements, in asymptotic kinematic and at CMC, were performed to have information about the surface activity of the components and the mechanical resistance of the interfaces. Data were interpreted by kinetic and rheological models, to know the interfacial characteristics of the investigated systems. To test the stabilizing effects of the polysaccharide, model emulsions were prepared using the investigated proteins and their stability was observed by creaming monitoring. The use of polysaccharides, in association with proteins, is very common in the food industry in order to stabilize products, so the study of the effects that polysaccharides have on VPs at the interfaces is important for the new product's formulation.

Tuesday 15:20 Virtual / Track 3 IR5

Viscoelastic properties of polyelectrolytes multilayers at the air/water interface

Stéphane Pivard[1], Leandro Jacomine[1], Gaël Ginot[1], Mélanie Legros[2], François Schosseler[3], Jean Farago[4], and Wiebke Drenckhan[1]
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Capsules of polyelectrolyte multi-layers (PEM) find increasing use in applications, ranging from the pharmaceutical to perfume sector. In many cases, fine control over the mechanical properties of the capsule shell is required, whose reliable characterisation remains an experimental challenge [1-2]. Here we produced multilayer capsules via layer-by-layer deposition of polyallylamine hydrochloride (PAH) and sodium polystyrene sulfonate (NaPSS) on an air bubble surface. Investigation of their viscoelastic properties by the classical Young-Laplace drop shape analysis is possible only for viscoelastic liquids. As soon as the PEM skin becomes a viscoelastic solid this analysis cannot be used because the stress is no longer homogeneous and isotropic [3-4]. We therefore present a method of determination of the dilational elastic modulus using a pressure sensor in parallel with sinusoidal deformation of the bubble (left Figure). We propose a representation of the pressure differential as function of area variation (A/A0). Fitting ellipsoidal figures resulting from smoothed data and finding the slope of their major axis (right Figure), we show that this parameter is related to the bubble radius, the pressure differential and the dilational elastic modulus. We investigated with this method the effect of strain rate, number of polyelectrolyte layers and bubble size. At last, we complement the results of this method with additional shear rheology to determine the mechanical properties of PEM materials of few nanometers thickness as successive NaPSS/PAH bilayers are adsorbed at air/water interface.

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Symposium MS

Modelling and simulations

Organizers: Natalie Germann and Daniel Read

Tuesday 13:20 Virtual / Track 4 MS1

A Lagrangian-Eulerian method for simulation of viscoelastic free-surface flows

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Viscoelastic flows appear in many industrial applications, including polymer extrusion, additive manufacturing, seam sealing and adhesive joining. Such applications may involve continuous inflow of a viscoelastic fluid from a nozzle, as well as complex and moving product geometry. These properties respectively increase the complexity of numerical modelling, as well as the involved computational cost, rendering industrial

problems difficult to simulate. In this work we present a simulation framework for viscoelastic free surface flow developed specifically to handle such flows. The fluid momentum and continuity equations are discretized with the finite volume method on an adaptive and dynamic octree grid. Furthermore, boundary conditions from objects in the domain are treated using an immersed boundary method. Complex moving geometries are therefore treated efficiently. The viscoelastic stresses are calculated with a recently proposed Lagrangian-Eulerian method, in which the constitutive equation is solved at Lagrangian nodes which are convected by the flow. A backwards-tracking methodology is used which allows for the storage of the viscoelastic stresses in relation to the Eulerian grid to be chosen a priori, enabling robust and efficient coupling between the velocity and stress fields. The viscoelastic free surface flow is treated using the volume of fluids method by solving the transport equation for the fluid volume fraction. For cases involving moving nozzles, the inflow of viscoelastic fluid is modelled with an injection model. The injection model is responsible for modifying the fluid volume volume fraction such that the correct inflow is prescribed, depending on the type of nozzle. The simulation framework is demonstrated for benchmark cases of viscoelastic free surface flows as well as for industrial scale robot-carried adhesive application.

Tuesday 13:40 Virtual / Track 4 MS2

Bubble Rise and Deformation in Elastoviscoplastic Materials

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Chemical Engineering, Fluid Mechanics and Rheology, University of Patras, Patras, Greece

The buoyancy-driven rise of a bubble through complex materials is a topic of great interest, relevant to various industrial sectors, such as oil drilling or food processing where bubble motion affects the efficiency the processes and the quality of the final product. Thus, a precise understanding of the dynamics of rising bubbles is of utmost importance. Therefore, we undertake a theoretical (computational) study of the transient rise of a single bubble, which starts translating from rest, inside an elastoviscoplastic material. The rheological behavior of the material is modeled with the use of the Saramito Hershel-Bulkley (SHB) constitutive equation [1]. The governing momentum and mass balance equations are solved numerically using the newly, developed finite element method for free surfaces by Varchanis et. al. [2], namely PEGAFEM-V. Furthermore, we assume axial symmetry, and the center-of-bubble volume remains at the origin of the coordinate system. By conducting transient simulations, we examine the steady-state shape and velocity of the bubble as well as the time evolution of its velocity for different bubble volumes. We have a very good agreement between the predicted shapes and terminal velocities compared with the respective experimental results of Lopez et. al. [3]. Our results indicate that for small bubble volumes, elasticity prevails, and the inverted teardrop shape is attained. As we increase its volume, the bubble obtains an oblate/spheroid shape, which is a typical manifestation of dominant inertia. Moreover, we perform a parametric study by varying several material parameters, e.g., the yield stress or the shear modulus. Our novel numerical results will help us elucidate further the peculiar bubble dynamics in elastoviscoplastic materials.

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Tuesday 14:40 Virtual / Track 4 MS3

Nonequilibrium thermodynamic modeling of multicomponent mixtures with partially miscible components

Ali Ghaemi and Natalie Germann
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Understanding the fluid dynamics of mixing systems with partially miscible components is of great importance in many industrial applications such as chemical purification and extraction. Based on the generalized bracket approach of nonequilibrium thermodynamics, we propose a phase field approach to describe multicomponent systems with different degrees of miscibility [1]. In this first phase of our research, we use a non-random multi-fluid type of local decomposition equation for the mixing energy to account for the non-ideal behavior of real mixtures [2]. We show that by expressing the generalized chemical potential by a nontrivial velocity difference between the components, we can avoid excessive diffusion and obtain more reliable results. We validate our numerical OpenFOAM implementation by solving the ascending bubble problem and compare our results with benchmark data from the literature [3-4]. We also successfully validate the implementation of our new phase field model under real flow conditions, i.e., with experimental observations made in a Y-shaped microchannel. We accurately predict the position of the interface and reproduce the mixing behavior of miscible and partially miscible components. This framework is very versatile; different forms of viscoelasticity, phase and state transitions, chemical or enzymatic reactions, and microorganisms can be easily accounted for in the near future.

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Tuesday 15:00 Virtual / Track 4 MS4

A CFD-DEM Eulerian-Lagrangian solver for particle-laden viscoelastic flows

Célio Fernandes[1], Salah A. Faroughi[2], Ricardo Ribeiro[1], João M. Nóbrega[1], and Gareth H. McKinley[2]
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The ability to simulate the behavior of dense suspensions using computationally-efficient Eulerian-Lagrangian techniques requires accurate particulate-phase drag models that are valid for a wide range of material parameters. The present work aims at developing appropriate drag models for moderately-dense suspensions, in which the continuous phase also has viscoelastic characteristics. To this end, we parametrize the suspension properties through the Deborah number and the particle volume fraction, and compute the evolution in the drag coefficient of spheres translating through a viscoelastic fluid that is described by the Oldroyd-B model. To calculate the drag coefficient, we resort to 3D direct numerical simulations (DNS) of unconfined viscoelastic creeping flows ($Re < 0.1$) past random arrays of stationary spheres, over a wide range of Deborah numbers ($De < 5$), volume fractions ($\varphi < 20\%$) and particle configurations. From these calculations we obtain a closure law $F(De, \varphi)$ for the drag force in the viscoelastic fluid (with fixed retardation ratio $\beta = 0.5$), which is on average within 4.7% of the DNS results. Subsequently, this closure law was incorporated into a CFD-DEM Eulerian-Lagrangian solver to handle particle-laden viscoelastic flow calculations, and two case studies were simulated to assess the accuracy and robustness of our numerical approach. These tests consisted of simulating the settling process in Newtonian and viscoelastic fluids within eccentric annular pipes and rectangular channels; configurations commonly employed in hydraulic fracturing operations. The numerical results obtained were found to be in good agreement with experimental data available for suspensions in Newtonian matrix fluids. For the case of viscoelastic fluids, the resulting particle distribution is presented for different elasticity numbers (i.e., $El = De/Re$) and particle volume fractions, and the results provide insight into the pronounced effects of viscoelastic matrix fluids in hydraulic fracturing operations.

Tuesday 15:20 Virtual / Track 4 MS5

Numerical investigation of particle motion in rheometric flows of non-colloidal suspensions

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The current work aims to investigate numerically particle movement taking place in rheometric flows. The proposed model is based on a two-fluid model that considers averaged mass and momentum equations for each phase and includes constitutive equations for drag, virtual mass, and lift forces to account for interphase interactions between solid and liquid phases. The equations are solved by using the Finite Volume ANSYS CFX software. The studied geometry consists of a 35 mm parallel-disk geometry separated by a 1 mm gap. A 3D solution domain is assumed, the disks are modeled as no-slip walls, with one rotating and the other static. The lateral interface between the sample and the ambient is modeled as a free-slip surface. Buoyancy is considered, the flow is assumed as isothermal and laminar and the phases are treated as particles dispersed in a yield stress fluid. The numerical results were corroborated with analytical solutions for liquid single-phase flows. The single-phase flow solutions revealed the existence of a second radial flow between the disks that influence the calculated torque at a given rotating Reynolds number. The secondary flow orientation, however, depends on which disk is rotating; while the fluid near the upper wall flows outwards when the upper disk rotates, the opposite occurs when the lower disk rotates. The two phase-flow simulations showed that the particle motion in non-buoyant flows is mainly driven by a combination of gravity and the secondary flow. Numerical experiments were conducted by rotating the upper or lower parallel plates and varying Reynolds and Bingham numbers. It can be summarized that the higher the Bingham number and the smaller the Reynolds number, the smaller the magnitude of secondary flow and consequently particle migration.

Symposium FB

Food and bio-rheology

Organizers: Jan Engmann and Clément de Loubens

Tuesday 13:20 Virtual / Track 5 FB1

Shape of rigid filaments determines the suspension dynamics and rheology

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We study how the shape of rigid filaments influences the dynamics and mechanical properties of their entangled semi-dilute suspension. To tune the filament shape we use bacterial flagella which are microns long helices assembled from flagellin monomers. We compare the dynamics of helical filaments and shape diblock copolymers with straight and helical segments to that of conventional rigid rods. Using single filament imaging we quantify how the filament shape affects the dynamics of semi-dilute suspensions. Straight filament, caged by its neighbours, easily diffuses along their its long axis, but exhibits significantly suppressed rotational diffusion. Helical filaments entangle much more easily when compared to equivalent straight rods. They can escape their confining tube only by corkscrewing through the dense obstacles created by other filaments. The two segments of the rod-helix block copolymers exhibit incompatible dynamics and thus become permanently jammed at exceedingly low volume fraction. We relate microscopic dynamics of individual filaments to macroscopic rheological properties of their suspensions. In particular, experiments show that entangled suspensions of shape block-copolymers at very low concentrations behave as soft solids, although they are missing any specific chemical links. The magnitude of their elastic moduli can be predicted from single filament dynamics. Our results demonstrate how tuning the shape of the constituent rigid filaments can be used to engineer the rheological properties of entangled rigid filament suspensions.

Tuesday 13:40 Virtual / Track 5 FB2

Erythrocyte sedimentation rate : collapse of a high volume fraction soft colloidal gel

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Red blood cells (or erythrocytes) sedimentation rate (ESR) is a physical parameter of blood which is often checked in medical diagnosis. It is indeed well known that in case of inflammation, the increase in fibrinogen and other proteins induces a higher ESR. Until now, researchers thought that the increase of fibrinogen accelerates the ESR by creating bigger aggregates of red blood cells (RBC). Fibrinogen is indeed an aggregation agent of RBCs, and bigger aggregates tend to sediment faster in Stokes regime. However, modeling the ESR measurements with this hypothesis is challenging and often requires physical assumptions specific to this system. Besides, modern colloidal science has shown that attractive particles form percolating aggregates, as wide as the container. The sedimentation of those colloids then follows a so-called "colloidal gel collapse" regime. Here, we show that RBCs actually follow the same behavior. We present detailed measurements of experimental ESR curves, and original micro- and mesoscopic pictures supporting this claim. Besides, those experimental observations are supported by 2D and 3D numerical simulations. We also demonstrate that such assumption naturally leads to efficient analytical modeling for the sedimentation curve of RBC.

Tuesday 14:40 Virtual / Track 5 FB3

Buffered λ-DNA solutions at high shear rates

Haider Dakhil[1], Santanu K. Basu[1], Silvia Steiner[1], Yasmin Gerlach[1], Alexander Soller[1], Sharadwata Pan[2], Natalie Germann[2], Maria Leidenberger[4], Barbara Kappes[3], and Andreas Wierschem[1]
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We study buffered aqueous solutions of λ-DNA at shear rates up to 10^5 s^{-1}. The shear rates are accessed with a narrow-gap rheometer at gap widths down to 20 µm [1-3]. At lower shear rates, our data merge with literature values. At high shear rates, the viscosity levels off into an infinite-shear viscosity plateau that hardly differs from the solvent viscosity. In the semidilute unentangled regime, we find that the DNA contribution to the viscosity obeys a power law with an exponent of about -0.36.

For the normal stress differences, we observe a power-law dependence on the shear rate up to shear rates of about 10^4 s^{-1}. Beyond this shear-rate range, we observe a stepwise change with the shear rate. While we do not find fragmentation of the λ-DNA, at shear rates beyond about $3\cdot 10^4$ s^{-1}, i.e. in the second plateau of the normal stress differences shear-induced changes of the DNA appear.

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Tuesday 15:00 Virtual / Track 5 FB4

Single red blood cell dynamics in time-dependent microfluidic flows

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Blood is mainly comprised of red blood cells (RBCs) that determine the unique flow properties of blood in the circulatory system. Their high deformability allows them to squeeze through microvessels much smaller than their equilibrium size. In microfluidic flows with channel dimensions similar to their size, RBCs exhibit characteristic shapes, such as croissants and slippers, depending on their confinement, velocity, and initial conditions. Although RBCs have been studied under steady flow conditions, knowledge about their flow behavior and shape transitions in unsteady flows remains vague. In this study, we perform microfluidic experiments in combination with numerical simulations to examine single RBCs in time-dependent flow fields. We use a high-precision pressure device to generate an unsteady driving of the flow in the microchannels and track single cells along the channel flow direction in a comoving frame. Applying an increasing pressure ramp, we find that the transition from the croissant to the slipper shape is faster than the opposite shape transition at a decreasing pressure ramp. Further, we observe that slipper-shaped RBCs oscillate laterally towards the sidewalls while traveling through the microchannel. The frequency of these oscillations increases with the cell velocity and with the viscosity of the surrounding fluid. Our study aims to understand how the time scale of the flow couples with the characteristic time scale of single RBCs in capillaries.

Tuesday 15:20 Virtual / Track 5 FB5

Microrheology of a cyanobacterial extracellular polymer in human blood plasma

Tomás Rodrigues[1], Rita Mota[2], Luís Gales[3], Paula Tamagnini[4], and Laura Campo-Deaño[1]

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Cyanoflan is a sulfated Released PolySaccharide (RPS) produced by a particular marine cyanobacterial strain [1]. This secreted extracellular polymer is rather complex structurally, being mainly composed by carbohydrates but also by sulfated residues and proteins. The apparently stochastic nature of the synthesised polymeric networks explains the palette of molecular masses that characterises *Cyanoflan*, as high as 2 MDa. The polymer proved suitable for a number of biotechnological applications: from emulsifying/thickening agent in food or cosmetic industries to drug delivery carrier. To assess the viability of the latter, the viscoelastic properties of this naturally secreted cyanobacterial polymer were evaluated at different concentrations in human blood plasma using microrheology. The multi-concentration analysis was instrumental in understanding how the RPS impacts the linear viscoelasticity of the biofluid *e.g.* enabling the identification of the sol/gel transition—or gel point—region (viscous liquid ⇔ gel), in terms of both Mean-Squared Displacement (MSD $\propto \tau^{\alpha}$ with $0 < \alpha < 1$; τ is lag time) and viscoelastic shear moduli ($G' \sim G''$ crossover). Ultimately, passive microrheology via Multiple Particle Tracking (MPT) made possible to determine a threshold concentration of cyanobacterial polymer beyond which a significant change of the microstructure of blood plasma takes place. This investigation endorses the study of *Cyanoflan* as a carrier for drug delivery, quantifying reasonable dosage limits in plasma from a rheological standpoint.

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Symposium ER

Experimental methods and rheometry

Organizers: Christian Clasen and Mariana Rodriguez Hakim

Tuesday 13:20 Virtual / Track 6 ER1

Simulated mechanical ageing of high voltage offshore windfarm power cables

David M. Hoyle and Alex Neumann

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It is now commonplace to see media stories about the green economy of the drive to net zero, with the offshore wind a key sector in providing clean energy in the future. To increase capacity and access stronger more frequency wind we need to go into deeper waters, and this requires floating turbines. Now floating and free to undulate, these floating wind turbines will put a huge strain on the power array cables that carry electricity to land. These high voltage power cables are an essential part of offshore energy operations and can operate at temperatures in excess of 90°C, making the insulating polymers becomes soft and malleable. Power cables are already the most common cause of turbine downtime costing millions of pounds to repair and that's before we consider the extra strain that the floating turbines will place on them. In my talk I will gives details of two Innovate funding projects that aim to test and solve some of these issues. Firstly, to test the effect of prolonged large amplitude oscillations on HV array power cables we have commissioned a Cable Bend Test mechanical analyser. Standing around 4m tall, the rig is capable of oscillating and stretching cables heated by electrical currents seen in wind turbines. By setting an oscillation amplitude and bend radius, we can measure the bending force going through the cable and simulate the ageing a cable will see in service. Secondly, if cable outer protective sheath is damaged, we are working with Kinectrics, who are developing a water activated expanding layer that can swell into this area of damage and protect the cable from water ingress. We are currently investigating the effectiveness of this hydrophilic thermoplastic elastomer layer using a bespoke high-pressure testing vessel. The key to both projects, is to identify the correct analysis techniques that most accurately characterises the age of the cable.

Tuesday 13:40 Virtual / Track 6 ER2

Dynamic mechanical analysis with torsional rectangular geometry: A critical assessment of constrained warping models

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Dynamic mechanical oscillatory shear measurements with torsional rectangular geometry are widely carried out in order to determine the mechanical properties of soft solid materials in a quick and practical way. This technique has the advantage of avoiding slip effects, thus being particularly attractive for testing stiff elastomers such as vulcanized rubber compounds. However, one of its drawbacks is the clamping system required to keep the specimen edges in place. Since it imposes a constraint to warping deformations (i.e., out-of-plane cross-section distortions about the torsional axis), a certain increase of dynamic moduli with respect to their values in simple shear is observed and considered as an experimental artifact (i.e., de Saint-Venant's assumption of primary torsion of the specimen is no longer valid). The increase of dynamic moduli in torsion depends on the specimen's cross-section geometry and relative dimensions. We test here the capability of different torsion models to describe the constrained warping effect for an industrial rubber with rectangular specimen cross-section using a wide range of different geometric parameters (length-to-width p ratio and width-to-thickness u ratio). We compare two theoretical models (Vlasov's model and Timoshenko's approach) and a phenomenological model (based on finite element simulations by Diani and Gilormini) with our experimental data set. We propose a slight modification of Vlasov's model to obtain realistic predictions of torsion over a wider parameter range. It is shown to be particularly useful in soft rubber testing, and the limitations in the choice of specimen geometry to obtain sufficient torque signal are overcome.

Tuesday 14:40 Virtual / Track 6 ER3

Properly designing capillary viscometry tests of molten polymers that slip through freely available software

Lorenzo Malagutti, Francesco Mollica, and Valentina Mazzanti
Engineering, University of Ferrara, Ferrara, Ferrara 44122, Italy

The measurement of viscosity of polymeric melts that slip at solid walls is troublesome. The Mooney procedure is one of the most common methods to quantify slip and thus to correct for obtaining reliable measurements. On the other hand, it can lead to significant error amplifications, giving rise to errors that may even yield unphysical results. This is especially true in the case of concentrated polymeric suspensions, e.g. heavily filled polymer melts or molten wood plastic composites. In this work, we study these issues analytically. As a test model, we decided to use a power law fluid and a slip constitutive equation also following a power law, but with an exponent that is the reciprocal of that of the flow rule. Two software programs have been developed. The first software quantifies the error amplification, the other one can be used by researchers for properly designing the testing setup. Both programs are freely available in the Mendeley Data Repository. As a first result, we showed that the uncertainty on the capillary radius is the main parameter that influences viscosity measurement accuracy. The main finding, however, is that lower accuracy can be the result of a higher shear thinning fluid behavior. Moreover, if the fluid has a high viscosity and slips at the wall easily, it is very difficult to obtain an accurate viscosity measurement: fluid kinematics here is obviously more dependent on slip properties rather than viscosity. In any case, radius tolerance must be very narrow to achieve reliable characterization.

Tuesday 15:00 Virtual / Track 6 ER4

Rheometric advances to cover the maximum possible range in temperature and frequency in a single measurement

Andre Braun[1], José Rodríguez Agudo[1], Andreas Westphal[2], and Jörg Läuger[1]
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Covering the widest possible range in temperature and frequency during a single measurement is a challenge in modern rheometry. The classic solution is to find a compromise between the properties of the material and the measurement system to be used. This can be especially difficult when the material undergoes a drastic change in its properties during the measurement (e.g., it experiences softening after the glass transition temperature (T_g)). If the sample is stiff at temperatures below T_g (G' above typically 1 GPa), we usually tend to use plates with a small diameter. This is necessary to prevent the equipment's own torsional compliance from affecting the results. However, this diameter may not be adequate when the module is very small (well above T_g). Similarly, if we want to measure at high frequencies (up to 102 Hz), a logical tendency would be to use a Separated Motor Transducer (SMT) system to avoid problems with inertia. However, in this scenario, the effect of torsional compliance is greater and therefore may not be adequate when the sample is stiff. In this contribution, we present a rheometric strategy to cover the possible maximum range in temperature and frequency in a single measurement. The solution is based on an SMT system working with a plate-plate geometry. Accurate knowledge of the instrument compliance is required to compensate the torsional compliance when the sample is stiff. In addition, a novel control system was specifically optimized for this task. We present different application examples. In the case of pressure-sensitive adhesives (PSA), the equipment is capable of performing correct measurements up to frequencies of 102 Hz, at temperatures between -80°C and 200°C. The reliability, precision and robustness of the measurements were tested in multiple rheometers. In other examples, the equipment was able to cover up to 9 orders of magnitude in G' during a single measurement.

Tuesday 15:20 Virtual / Track 6 ER5

Towards a universal shear correction factor in filament stretching rheometry

Frank P. A. van Berlo, Ruth Cardinaels, Gerrit W. Peters, and Patrick D. Anderson
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Filament stretching rheometry is a prominent experimental method to determine rheological properties in extensional flow whereby the separating plates determine the extension rate. In literature several correction factors that can compensate for the errors introduced by the shear contribution near the plates have been introduced. In this work a systematic analysis is conducted to determine if a material-independent correction factor can be found for non-linear viscoelastic polymers. To this end a finite element model is presented to describe the flow and resulting stresses in the filament stretching rheometer. The model incorporates non-linear viscoelasticity, and a radius-based controller is added to mimic the typical extensional flow in filament stretching rheometry. The model is validated by comparing force simulations with analytical solutions. The effects of the end-plates on the extensional flow and resulting force measurements are investigated, and a correction factor in the non-linear viscoelastic flow regime is determined. This correction factor shows good agreement with simulations performed at multiple aspect ratios and strain rates and is shown to be valid for a range of polymer melts with non-linear rheological behaviour.

Symposium PM

Polymer melts and composites

Organizers: Maria Teresa Cidade and Juan de Vicente

Tuesday 13:20 Virtual / Track 7 PM29

Assessment of transient shear response of entangled polymers

Daniele Parisi[1], Emmanouil Vereroudakis[1], Yuichi Masubuchi[2], Giovanni Ianniruberto[3], Giuseppe Marrucci[3], and Dimitris Vlassopoulos[1]

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Whereas the shear stress overshoot of entangled polymers is established, experimentally and theoretically, other features of the transient response remain debatable. In particular, a weak undershoot has been reported to often proceed the eventual steady state. However, this was not always systematically observed. On the other hand, modeling approaches can provide a rationalization of the undershoot by invoking the idea of tumbling which itself stems from simulation results. This is not universally accepted yet. Here we aim at providing further evidence in the direction of clarifying the issue as much as possible and in particular identifying experimental and molecular conditions or parameters (based on characterization of materials and flow geometry) for the appearance or not of undershoot.

Tuesday 13:40 Virtual / Track 7 PM30

Modelling the linear viscoelastic behavior of unentangled associating polymer melts

Hongwei Liu and Giovanni Ianniruberto

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The Rouse model reasonably describes the linear viscoelastic behavior of unentangled melts of ordinary polymers [1], as well as of associating polymeric networks with reversible stickers [2]. Here, in order to attempt a quantitative comparison with more recent data [3], we develop a simulation algorithm accounting for the distribution of chain lengths (polydispersity), and of sticker position along the chains. We also aim at accounting for a distribution of sticker strength, with aim of describing the rheology of double-dynamics networks [4,5]. The simulation approach is also combined with a pseudo-analytical approach where the role of stickers is accounted for by assuming that the monomeric friction coefficient is not uniform along the chain.

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Tuesday 14:40 Virtual / Track 7 PM31

Temperature-controlled filament stretching during micro-extrusion of highly filled polymer suspensions

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Fraunhofer Institute for Solar Energy Systems ISE, Freiburg im Breisgau, Germany

For successful metallization of silicon solar cells, a metal grid with fine lines below widths of 30 µm is printed onto the solar cell surface. Parallel dispensing is an upcoming technology which allows the extrusion of a highly filled polymer-suspension through up to 150 parallel micro-nozzles. In order to further increase process speeds under stable conditions, a careful adaptation of the suspension rheology is crucial. Besides the optimization of the suspension formulation, the rheology can be adjusted by changing the suspension temperature during printing. Therefore, this study presents an experimental evaluation of the maximal attainable process speed by adjustment of process temperature. It is found that an increase in temperature promotes dynamic filament stretching between the nozzle exit and the contact point on the substrate. This effect allows to adjust the relative velocity between print head and paste extrusion, resulting in an increased production throughput as well as in a shrinkage of printed lines due to the dynamic stretching of the filament. This shrinkage of printed structures does not require a further reduction of nozzle openings and therefore bypasses the challenge of increased clogging whenever nozzle diameters are further reduced in extrusion processes of highly filled suspensions. The rate of stretching is investigated for different polymer-solvent combinations, temperatures, process speeds and nozzle diameters. It was possible to achieve an increase in process speed of up to 56% to 430 mm/s compared to the reference process at room temperature, resulting in a reduced, printed line width of 25 µm. The presented data highlights how a systematic control of the process temperature in industrial micro-extrusion processes of polymer suspensions can not only improve the process stability and throughput-rates but also further reduce the dimension of printed structures beyond the conventional limit without filament stretching.

Tuesday 15:00 Virtual / Track 7 PM32

From nano to microscale: the influence of the structure and morphology of the carbonaceous fillers on the rheological properties of polymeric composites

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It has been well known for many years that the addition of carbonaceous nanofillers has a strong impact on the mechanical, electrical, thermal and rheological properties of polymers. From of point view of rheological properties, different and ambiguous effects of the carbonaceous nanofillers on the rheological properties of the polymers have been reported. Some studies have shown that the carbonaceous nanofillers increase the modulus and the viscosity of the polymers. Other studies have shown that the nanofillers decreased the modulus and the viscosity of the polymers. Here, we evaluate the consequence of the incorporation of two-dimensional (2D) carbonaceous fillers, such as graphite (Gr), graphite oxide (GrO) and graphene oxide (GO) on the rheological properties of different polymers. In this study, we evaluated the consequence of the incorporation of the fillers in the steady shear viscosity behavior, the creep behavior and the linear viscoelastic properties of polymeric composites. The GrO was obtained by the chemical modification (Hummer's method) of Gr. Subsequently, the GrO was exfoliated in an ultrasound bath, obtaining the GO. The obtained results indicate that GO increases the modulus and the viscosity of the polymer, while GrO and Gr behave in a "lubricating way" for the polymer, reducing the viscosity and modulus of the polymer for high shear stress. The particles GO agglomerate have behaved similarly to the 3D material (GrO). These results indicate that depending of scale of the fillers, composites can present different behavior.

Tuesday 15:20 Virtual / Track 7 PM33

Janus rod stabilized polymer blends: the effect of entanglements on shear flow and relaxation behavior

Shaghayegh Khani[1], Felipe Paiva[2], Argimiro Secchi[2], Veronica Calado[2], and Joao Maia[1]
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Understanding the relationship between interfacial microstructure and rheological properties is paramount for design and processing of polymer blend materials with controlled morphologies. Janus nanorods as a new class of rigid surfactants have shown promising performance in compatibilizing polymer blends. Recent studies by our group have linked the interfacial microstructure of Janus nanorods with their interfacial properties and morphology of unentangled polymer blend systems. Herein, we use a segmental repulsive potential in the framework of Dissipative Particle Dynamics in order to capture dynamics and viscoelastic properties of entangled polymers. Shear flow and relaxation behavior of entangled polymer blends stabilized by Janus and homogenous nanorods are investigated to provide insight into the structure-property relationships. Shear induced microstructure may be stabilized by nanorods depending on their interfacial orientation. The effect of entanglements on morphological changes are traced back to the relaxation of normal stresses in such systems.

Symposium FI

Flow instabilities

Organizers: Sandra Lerouge and Mahdi Davoodi

Tuesday 13:20 Virtual / Track 8 FI1

Cutting and slicing weak solids

Serge Mora[1] and Yves Pomeau[2]
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Dicing soft solids with a sharp knife is quicker and smoother if the blade is sliding rapidly parallel to its edge in addition to the normal squeezing motion. We explain this common observation with a consistent theory suited for soft gels and departing from the standard theories of elastic fracture mechanics developed for a century. The gel is assumed to locally fails when submitted to stresses exceeding a threshold sigma_1. The changes in its structure generate a liquid layer coating the blade and transmitting the stress through viscous forces. Whether the deformations of the solid phase are large or small does not matter in the theory, the important property being that the gel remains elastic below a critical stress is reached. In that sense, the theory fundamentally departs from standard theories of fracture mechanics that are based on the calculation of elastic deformations together with an estimation of the energy release rate taking place in the plastic zone. The driving parameters in the model are the ratio U/W of the normal to the tangential velocity of the blade, and the characteristic length eta W/sigma_1, with eta the viscosity of the liquid. The cutting process is independent of the yield criterion of the gel. The model does predict that a thinner edge facilitates the cleavage. In addition, a symmetric cross section of the blade is found to be more efficient than a bevel. The existence of a maximal value of U/W for a steady regime explains the crucial role of the tangential velocity for slicing biological and other soft materials.

Tuesday 13:40 Virtual / Track 8 FI2

Yielding of a paraffin wax to heat: a focus on the hydrodynamic stability

Rawad Himo, Cathy Castelain, and Teo Burghelea

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Microstructured materials typically yield when subjected to an external forcing able to disrupt their microstructure. Whereas a significant progress has been made towards understanding the yielding to stress, much less is understood in the case when a material loses its micro-structural integrity due to heat(ing). We focus here on the yielding of a commercial paraffin wax subjected to a controlled external heating during a rheometric flow. As one would expect, a gradual heating of the wax translates into a transition from a solid state to a fluid one. Yet, by careful time resolved measurements of the apparent viscosity combined with in-situ visualisations of the dynamics of the micro-structure we show that this yielding process triggered by heat is accompanied by a break-down of the hydrodynamic stability of the system: melting during flow is a genuinely unstable physical process. We provide a full description of the hydrodynamical instability observed near the melting point. Based on numerical simulations performed on a simple toy model, we propose a phenomenological picture of this novel instability.

Tuesday 14:40 Virtual / Track 8 FI3

Mechano-optical characterization of extrusion flow instabilities in styrene-butadiene rubbers: investigating the influence of molecular properties and die geometry

Christos K. Georgantopoulos[1], Masood K. Esfahani[1], Carlo Botha[1], Ingo Naue[1], Nico Dingenouts[1], Andrea Causa[2], Roland Kádár[3], and Manfred Wilhelm[1]

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The extrusion flow instabilities[1] of two commercial styrene-butadiene rubbers (SBR) are investigated as they vary in isomer content (1,4 cis, 1,4 trans and 1,2 conformation) of the butadiene monomer and the molecular architecture (linear, branched). The investigated samples have similar multimodal molecular weight distribution (MWD). Two geometries of extrusion dies, slit and round capillary, are compared in terms of the type and the spatial characteristics of the flow instabilities. The latter are quantified using three methods: a highly pressure sensitive slit die,[2] online and offline optical analysis.[3] The highly pressure sensitive slit die has three piezoelectric pressure transducers placed along the die length. The characteristic frequency of the flow instabilities follows a power law behavior as a function of shear rate to a 0.5 power for both materials. A qualitative model is used to predict the spatial characteristic wavelength (λ) of the flow instabilities from round capillary to slit dies and vice versa. Slip velocities (Vs) are used to quantify the slippage at slit and round capillary dies as well.

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Tuesday 15:00 Virtual / Track 8 FI4

Symmetry breaking of a parallel two-phase flow in a finite channel

Paul R. Kaneelil[1], Amir A. Pahlavan[1], Miguel A. Herrada[2], Kristen LeRoy[3], Kylie Stengel[3], Samuel Warner[3], Anna M. Galea[3], and Howard A. Stone[1]

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Parallel two-phase flows are omnipresent in technological applications that require contact between two immiscible fluids for a finite amount of time. Precise control over the flow and separation of the fluids once they have been in contact are therefore the key challenges in these applications. Here, we report on the surprising observation that the parallel two-phase flow of fluids with equal viscosities and flow rates in a symmetric device leads to an interfacial instability at the exit junction, preventing perfect separation of the two fluids. This instability leads to a periodic shedding of droplets, the period of which is inversely proportional to the flow rate. Varying the geometric features of the system and the flow rates of the two fluids, we show that the instability is never suppressed. We argue that trace amounts of surfactants that are present in any system can accumulate at the interfacial stagnation point at the exit junction, creating a Marangoni backflow along the interface, leading to symmetry breaking and the instability of the interface.

Tuesday 15:20 Virtual / Track 8 FI5

Displacement flow of a yield stress fluid from an eccentric annulus by a turbulent wash

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We study displacement flows in strongly eccentric annuli, where the in situ fluid is viscoplastic and the displacing fluid is Newtonian. This mimics the situation found in the cementing of horizontal oil and gas wells. In this configuration, it is common that the yield stress of the displaced fluid prevents displacement from the narrow side of the annulus, where it remains static. We address the question of whether a turbulent flow of the displacing fluid will be effective in removing the static narrow side channel and by what means. Using Carbopol and mostly water to displace, a range of experiments have been performed in a horizontal laboratory annulus. The flows proceed with rapid displacement along the wide side of the annulus, leaving behind a gelled channel of fluid on the narrow side. The narrow side is displaced either slowly or not at all. We show that secondary flows in the turbulent displacing fluid are essential to the displacement. We study a range of effects: drag reducing polymers, buoyancy effects, using viscous laminar fluids, etc., all in comparison to the water. The main conclusion is that yield stress fluids in highly eccentric annuli are very difficult to remove.

Symposium MP

Multiphase and other complex fluids

Organizers: Mario Minale and Dganit Danino

Tuesday 13:20 Virtual / Track 9 MP1

Modeling vorticity stretching of viscoelastic droplets during shearing flow

Abdulwahab S. Almusallam[1] and T.B. Bini[2]

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In the present work we are focusing on the large deformation of a viscoelastic droplet suspended in a Newtonian matrix. We use the constrained volume model as a basic theoretical framework for the description of droplet shape evolution, and we account for the viscoelasticity of the droplet phase using the single-mode Giesekus model. The velocity gradient term describing flow inside the droplet is modified by the viscoelastic stresses, and the resulting model - we herein call the non-Newtonian Constrained Volume model (nN-CV model) - is calibrated by matching its predictions to those of the model of Yu, Bousmina, Zhou and Tucker (YBZT model) [J. Rheol. 48, 417-438 (2004)] at small deformation and slow flow conditions. The nN-CV model is then examined under conditions of large deformation and/or fast flow, and its predictions are compared against experimental results available in the literature. The new model is able to show vorticity growth at conditions of large capillary and elastocapillary numbers. Its predictions are studied by the visualization of flow inside the droplet and the analysis of polymer stresses inside the droplet.

Tuesday 13:40 Virtual / Track 9 MP2

Sheared droplets filled with non-Brownian particles: Particle distribution and droplet dynamics

Helene Van Ammel[1], Joana Ferreira[2], Simon Kuhn[2], Paula Moldenaers[1], and Ruth Cardinaels[1]

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Droplets encapsulating particles can be encountered in various application areas such as the oil, printing and food industries. To study the flow-induced dynamics of droplets containing non-Brownian particles, single particle-filled droplets are visualized in a counter-rotating shear flow cell. The particle over droplet size ratio (r/R) is changed by using different particle sizes (r/R = 0.02-0.4). Additionally, the effect of particle concentration (5-20 vol%) is investigated for systems with a viscosity ratio either above or below 1 (0.09 and 1.4). For small r/R, the droplet phase can be considered as a homogenous medium characterized by its bulk viscosity which is governed by the particle concentration. Thus, the dynamics of droplets with r/R = 0.02 show good agreement with a particle-free reference system with a viscosity ratio comparable to that of the particle-filled system. However, droplets with r/R = 0.1 show a more suppressed deformation and slower transient dynamics and, therefore, behave as a slightly more viscous medium than expected based on their bulk viscosity. These effects become more pronounced at high particle concentrations, high r/R and for the viscosity ratio above 1. At particle concentrations above 15 vol%, local particle effects introduce qualitatively different droplet dynamics like asymmetric or oscillating droplet shapes and tip streaming. Finally, the particle distribution inside the droplets is analyzed. In shear flow, the particles migrate in the vorticity direction, whereby the viscosity ratio determines whether they accumulate around the equatorial plane or move away from it towards the sides of the droplet. In order to identify the flow profile and shear rates to which the particles inside the droplet are subjected, the particle-free droplet-matrix system is numerically simulated using the Volume-of-fluid method. Thereby, the observed particle distributions can partially be explained by shear-induced migration towards zones of low shear rates and low streamline curvature.

Tuesday 14:40 Virtual / Track 9 MP3

Numerical simulation of the coalescence-induced polymeric droplet jumping on the superhydrophobic surfaces

Kazem Bazesefidpar, Luca Brandt, and Outi Tammisola

Flow and Serc, Engineering Mechanics, Kth Royal Institute of Technology, Stockholm, Sweden

The coalescence-induced droplet jumping on superhydrophobic surfaces has received much attention in recent years due to its several industrial applications, including self-cleaning surfaces, anti-icing, and enhanced heat transfer. The influence of the surface wettability and droplet properties on the self-propelled jumping of the droplet has been investigated both numerically and experimentally. However, the influence of rheological properties on the self-propelled jumping, such as the polymeric relaxation time and polymeric viscosity ratio, has not been investigated to the best of our knowledge.

We present the implementation and performance of an efficient viscoelastic two-phase flow solver for the Cahn-Hilliard phase-field model incorporating moving contact line. The method uses a second-order finite difference method for the discretization of the fully coupled Navier-Stokes and Cahn-Hilliard model; and an efficient FFT-based solver is used for solving the equations. The Oldroyd-B model is used to model the viscoelasticity. We investigated the mechanism of selfpropelled jumping of the polymeric droplets by using three-dimensional simulation of two identical droplets on the surface with contact angle 180 degree. The numerical simulation is able to capture the spontaneous coalescence and

jumping of the droplets. The influence of elasticity and polymer viscosity ratio on the jumping process is investigated at different Ohnesorge numbers.

Tuesday 15:00 Virtual / Track 9 MP4

Can short, unentangled polymers be effective (self)compatibilizers in polymer blends?

Avanish Bharati, Ruth Cardinaels, and Paula Moldenaers
Soft Matter, Rheology and Technology, KU Leuven, Heverlee 3001, Belgium

Polymer blending offers an efficient strategy to develop materials with optimal properties superior to those of the components. By varying the polymers, the blend composition and processing routes, blends with a wide range of morphologies can be generated for tuning the final properties. Paradoxically, the inherent immiscibility of most polymers mandates their compatibilization to refine and stabilize the biphasic morphology. The classical strategy to improve the blends compatibility is the incorporation of premade block polymers. More recently, compatibilzation by nanoparticles has proven to be a successful alternative route. Here we describe a novel compatibilization strategy by employing novel compatibilizers, in particular short unentangled poly(styrene) (PS) polymers, in phase separating poly[(methyl styrene)-co-acrylonitrile]/poly(methyl methacrylate) (PMSAN/PMMA) blends or immiscible PS/PMMA blends. The compatibilization effectiveness of the PS polymers is assessed by in-situ characterization of the matrix-droplet morphology as a function of coalescence time using a flow-induced coalescence protocol. Below the entanglement molecular weight (Me), there is good compatibilization, discerned from both the decrease in the interfacial tension and the increase in the extent of coalescence suppression of the PMMA droplets in 85/15 PMSAN/PMMA and PS/PMMA blends. However, compatibilization significantly decreases if the molecular weight (Mw) of the PS polymers is increased above Me. The compatibilization effects are independent of the functionalization of the PS terminal groups and also hold when the compatibilizer has exactly the same chemical composition as one of the blend components, thus demonstrating the occurrence of self-compatibilization.

Tuesday 15:20 Virtual / Track 9 MP5

Study of bubble rising dynamics and interfacial scalar transport in Carreau-Yasuda quiescent fluid model

Koorosh Kazemi, Salvatore Cito, Alexandre Fabregat, and Vernet Anton
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Bubble rising in quiescent complex fluids is observed and/or induced in several natural, industrial and biochemical processes. Therefore, the control of the transport phenomena from the bubble into the fluid and predicting an accurate mass transfer rate is highly desired, especially in non-Newtonian fluids. Correlations between Sherwood and Peclet numbers are often used to control and understand the heat and mass transfer rates. However, such correlation is mainly established for spherical rigid bubble with clean surface rising steadily in quiescent fluids while for the given values of Bond and Galilei numbers, the trajectory of the bubble is time dependent, and the evolution of the bubble shape cannot be defined by its initial spherical shape. The complexity of the trajectory and the time evolution of the shape of the bubble plays an important role on the mass transfer phenomenon. Furthermore, shear dependent viscosity can farther alter the bubble rising dynamics with an explicit impact on the mass transfers phenomenon especially at high Peclet numbers.In the present study, we choose Bond number Bo=2, and Galilei number Ga=30 which are the border line values between a steady rising bubble and an oscillating rising bubble in Newtonian fluid. Within this transition zone, we explore the heat and mass transfer in shear thinning and shear thickening fluids imposing viscosity index values in-between 0.3 and 1.7 and Peclet number values in between 10 and 1000. The very thin and moving boundary mass transfer layer requires very refined computational mesh and very small time steps. To overcome these numerical complications, we model the two-phase flow fluid dynamics using volume of fluid methods together with octree methods to refine the mesh only around the bubble interface using an open solver, Basilisk. We extend the correlation between Sh and Pe to a wider range of cases including fluids with complex rheological behavior considering the non-sphericity of the bubble.

Symposium PG

Powder rheology, granular flows and rheology of solids

Organizers: Alexandra Aulova and Stefan Gstöhl

Tuesday 13:20 Virtual / Track 10 PG1

Interplay of gravitational and inter-particle forces in granular rheology

Thomas Voigtmann and Olfa D'Angelo
Institute of Materials Physics in Space, German Aerospace Center, Cologne, Germany

The rheology of dense granular systems displays a rich phenomenology: a dynamical yield stress and a shear-thinning regime are observed at low shear rates, reminiscent of glass-forming colloidal suspensions; at high shear rates, an inertia-dominated regime first identified by Bagnold appears. The stationary stress as a function of shear rate (i.e., the flow curve) can, depending on system parameters, evolve non-monotonically, indicating the tendency of the system to form spatially inhomogeneous, shear-banded flows. We study the influence of the dominant forces at play on the grain level, on these peculiar features of the non-monotonic flow curves. Experiments on polystyrene and metal powders and DEM simulations that mimic the cylindrical Couette-cell geometry of the experiments, are in good qualitative agreement. In particular, we discuss how the interplay between gravity and surface-roughness forces determines the typical shear rate and size of shear bands. The results give insight into the flow behavior of granular materials in the context of space-related applications such as powder handling and 3D printing in reduced gravity.

Tuesday 13:40 Virtual / Track 10 PG2

From powder rheology to 3D printing in space - and back

Olfa D'Angelo, Wolf T. Kranz, Thomas Voigtmann, and Andreas Meyer
Institute of Materials Physics in Space, German Aerospace Center, Cologne, Germany

As human reach into space expands, the need arises for triggering and controlling powder flow under unusual conditions − notably, in absence of gravity. This poses a major challenge for predicting and implementing reliable powder-handling processes in extreme environments such as planetary surfaces, satellites or spaceships.

We explore the links between the rheological properties of powders, measured under well-controlled conditions, and powder flow in microgravity, relevant for the development of a gravity-independent additive manufacturing process for space application.

Experiments on parabolic-flight, enabling to access varying gravity level, show that for dense flows, gravitational forces can drastically alter the force balance that determines the emergence of long-ranged force chains and leads to jamming, with dramatic consequences for the powder handling in reduced gravity. Using polystyrene particles modified to have rough and smooth surfaces, steady-state flow curves allow to observe and quantify the essential differences in powder-flow behavior that emerge from different surface properties of the grains, and hence the direct particle interactions. We finally demonstrate how the results from these experiments lead to the design of a novel powder-based additive manufacturing process that works independently of gravity, underlining the crucial link between rheological characterization of the powder base-material and the quality of the final printed part. The process has been implemented in a 3D printer that allowed to deposit and sinter homogeneous layers of granular materials of vastly different flow properties under weightlessness conditions. Using an in-situ probing mechanism, we observe the change in rheological response undergone by the powder feedstock as it is handled under different gravitational environments.

Tuesday 14:40 Virtual / Track 10 PG3

Insights into the rheology of cohesive granular media

Sandip Mandal, Maxime Nicolas, and Olivier Pouliquen
IUSTI, Aix Marseille University, CNRS, Marseille, France

Powders are widely handled in industries like pharmaceutical, food, cement, and so on, and often present challenges to these industries due to their poor "flowability". Therefore, characterization and prediction of the "flowability" of powders are of paramount importance to these industries. Although the static behaviors of powders are well-understood, there is less understanding of their dynamic behaviors, which is the focus of our study. Employing intensive discrete numerical simulations of cohesive grains (a prototype of powder) flowing down an inclined plane, we provide crucial insights into the flow behavior of powders. We show that unlike in the case of cohesionless grains, the rheology of cohesive grains is significantly affected by the stiffness and inelasticity of the grains − for the same inter-particle adhesion, stiffer and less dissipative grains yield a less cohesive flow. This observation is rationalized by introducing the concept of a dynamic, "effective" adhesive force, a single parameter, which combines the effects of adhesion, elasticity, and dissipation. Based on this concept, a rheological description of the flow is proposed for the cohesive grains. Our results elucidate the physics controlling the flow of cohesive granular materials, which may help in designing new approaches to characterize the "flowability" of powders.

Tuesday 15:00 Virtual / Track 10 PG4

Flow curves from granular materials inside a fluidized bed: experiment and theory

Matthias Sperl, Olfa D'Angelo, and Wolf T. Kranz
MP, DLR, Cologne, Germany

We measure the flow curves of granular particles agitated inside a fluidized bed shear cell from Anton Paar. The flow curves obtained are compared with the gMCT-ITT predictions for hard-sphere systems with dissipation [1]. Experiment and theory compare very favourably. Over several orders of magnitude, we observe three regimes for subsequently higher shear rates:

(1) Newtonian rheology for small shear rates,
(2) shear thinning for shear rates above the intrinsic relaxation rate for the granular fluid given by glassy dynamics of the system agitated by within the fluidized bed, and
(3) a shear thickening regime know as Bagnold scaling where the shear stress depends only on the time scale of the imposed shear rate.

Above a critical packing fraction identified with a granular glass transition [2] and low enough shear rates, a finite yields stress is observed.

An interpretation also in terms of traditional laws of granular rheology shall be provided [3].

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Tuesday 15:20 Virtual / Track 10 PG5

Control of a frictional fluid and plug formation in confined geometry

Louison Thorens[1], Mickaël Bourgoin[2], Stéphane Santucci[2], and Knut Jørgen Måløy[1]
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Multiphase flows involving the transport of granular material in confined geometries are crucial for industrial engineering processes, such as the transport of oil, water and sand in pipelines. They display a rich variety of instabilities leading to the formation of complex patterns stemming from the interplay of different physical processes, involving pressure and capillary forces, associated to frictional interactions inside the granular packing. Therefore, a clear understanding aiming at a control of such frictional fluid appears really challenging.

We investigate here, both experimentally and theoretically, a simple model system of a confined, multiphase frictional flow. A mixture of glass beads (few hundred microns size) in a Newtonian liquid is slowly drained out at a constant rate (thanks to a syringe pump) from a capillary tube (2 mm diameter), with one side open to the air. The resulting advancing air-liquid meniscus may push and accumulate particles ahead, in a so-called "bulldozing" process, up to a clogging situation. At this jamming point, the stress against the capillary walls exerted by the granular medium, competes with the pore pressure at which air percolates through the granular assembly. This process repeats periodically leading to the formation of a plug trail along the tube.

We first study the onset of the "bulldozing" process by varying the system's parameters - density, surface tension, amount of particles- and identify the experimental conditions leading to the unstable dynamics and plug formation. Then, we perform experiments with ferromagnetic grains, which acquire a magnetic moment when submitted to a magnetic field, leading to tunable pair interactions. In these conditions, we show that we can trigger the "bulldozing" dynamics. Moreover, we also show that the external magnetic field impacts the final plug pattern along the tube by tuning the Janssen effect inside the granular packing, paving the way towards a tunable frictional fluid.

Symposium MN

Micro and nano fluidics and microrheology

Organizers: Anke Lindner and Laura Casanellas

Tuesday 13:20 Virtual / Track 11 MN1

Production of viscoelastic droplets with encapsulated particles in a microfluidic channel

Keshvad Shahrivar and Francesco del Giudice
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The generation of droplets in microfluidic devices finds various applications such as particle/cell encapsulation and colloidal crystal synthesis. In this context, despite the potential advantages arising from the use of non-Newtonian liquids, studies featuring viscoelastic droplet formation and particle encapsulation are either spare (the former) or missing (the latter). We have investigated the formation of xanthan gum droplets in Newtonian fluids in a hydrophobic T-junction microfluidic device with internal diameter of 100 µm. As the dispersed phase we used aqueous solutions of xanthan gum, while for the continuous phase mineral oil was used. We successfully obtained continues formation of xanthan gum viscoelastic droplet in the hydrophobic device. We observed transition to unstable droplet formation regime, in contrast to the Newtonian case, in which the transition point changed proportionally to the continuous phase flow rate and it was inversely proportional to the xanthan gum mass concentration. Droplet size showed linear relation with flow rate ratios at high capillary numbers but deviation from Newtonian case was observed for low capillary numbers in the squeezing regime. We also provide the first evidence of particle encapsulation using viscoelastic fluids in microfluidic devices. Distribution of number of particle per drop was dictated by the Poisson statistics due to stochastic particle loading. Our results suggest that viscoelasticity and shear-thinning characteristic of the dispersed phase play a substantial role in the instability observed during the formation of viscoelastic droplets in T-junction and, consequently, in the particle encapsulation.

Tuesday 13:40 Virtual / Track 11 MN2

Relaxation of confined microfluidic droplets

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We investigate the response of a non-wetting droplet, confined in the rectangular section of a microfluidic channel, to a local variation of the channel topography. The local confinement gradient, that can reversibly be induced in the channel with using a thermomechanical actuation, leads the droplet to deform in its center and gets a peanut-like shape. When the topography of the channel goes back to flat, the droplet relaxes to its plug-like shape minimizing its surface energy under the constraints imposed by the channel walls. During this relaxation process, the liquid contained in the central neck drains towards the extremities of the droplet. Interestingly, we observe that the neck profile is self-similar. By coupling a force balance in the dynamical menisci of the relaxing droplet with a volume conservation of the external phase that has to flow through the gutters, we manage to recover the time evolution of the relaxation process. This approach integrates the role of the non-linear viscous dissipation in the dynamical meniscus of the neck [1]. This work allows us to show that classical models incorporating capillary driving with viscous dissipation employing geometrical invariance, whether translation or rotation cannot describe the relaxation in the intrinsically 3-dimensional geometry of the studied system. By considering the 3D problem, a scaling model incorporating dominant dissipation within the droplet menisci, allows to capture the self-similar droplet dynamics. Such confined relaxation, ubiquitous in real systems, allowed us to go beyond symmetry- based models on interface relaxation.

[1] Bretherton, J. Fluid Mech., 1961

Tuesday 14:40 Virtual / Track 11 MN3

Shape-specific hydrodynamic coupling of microparticle pairs in confined Stokes flow

Rumen N. Georgiev[1], Nagaraj Nagalingam[1], Robert Leliveld[1], William E. Uspal[2], Johan T. Padding[1], and H. Burak Eral[1]
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Particles of all shapes and sizes flowing under confinement are present in applications across length scales: from blood flow through tissue capillaries to industrial-scale processes. A particle in flow is strongly coupled to its surroundings via hydrodynamic interactions, which determine its motion. Recently, through both experiments and simulations, we elucidated the trajectory of any single microparticle with at least one mirror plane in a Hele-Shaw cell [1]. However, separation on the basis of shape requires considering particle-particle coupling. To this end, we investigate the flow-mediated interactions in pairs of non-circular objects in a Hele-Shaw cell. Regardless of their exact shape and symmetry, particles do not move relative to each other, provided the formed pair itself is mirror-symmetric. Conversely, particles in asymmetric pairs interact hydrodynamically and their relative motion depends on both their shape and the distance between them. In general, particles repel each other at distances smaller than the cell height and this repulsion diminishes as the distance increases. Moreover, most pairs exhibit weak attractions at distances between two and five cell heights. Therefore, interacting pairs tend towards a unique equilibrium distance, which is shape-specific. This process is similar to the self-assembly of droplets into trains [2]. By combining experimental and numerical techniques we study the effect of shape on this equilibrium distance. Thus, we conclude that particles in flow should spontaneously assemble into one-dimensional flowing crystals regardless of their shape.

[1] Georgiev et al., PNAS, 117, 21865-21872 (2020). [2] Beatus et al., Chem. Soc. Rev., 46, 5620-5646 (2017).

Tuesday 15:00 Virtual / Track 11 MN4

Predicting droplet velocity in a Hele-Shaw cell

Benjamin Reichert[1], Isabelle Cantat[2], and Marie-Caroline Jullien[2]
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We study the motion of low viscous droplets in a Hele-Shaw cell, while it is pushed by an external phase of imposed flow rate, at low capillary numbers. In this regime, the droplet's mobility, defined as the ratio between the droplet velocity and the external phase mean velocity, evolves non linearly with the capillary number, a signature of the different dissipation mechanisms at play. We propose a model based on a power balance approach together with the integration of the full complex topography of the lubrication film. Experiments are performed with surfactant free air bubbles in fluorinated oil, and with surfactant laded fluorinated oil droplets in water. Remarkably, the model reproduces the experimental data without any fitting parameter, and shows that even small surface tension variations appearing locally, due to an accumulation of surfactant at the rear meniscus, are enough to strongly modify the droplet velocity.

Tuesday 15:20 Virtual / Track 11 MN5

Rheofluidics: measuring mechanical properties of droplets at high throughput

Matteo Milani[1], Stefano Aime[2], and David Weitz[3]
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The characterization of the mechanical properties of small droplets represents an important task for many issues present in different research areas. For example, cancer spreading is accompanied by a reorganization of the cytoskeleton related to changes in cell stiffness. Moreover, the production of microcapsules, become one of the most used candidates for encapsulating, transporting, and/or controllably releasing a wide variety of technologically active materials like agricultural chemicals, food additives, and pharmaceuticals. Well-developed techniques like AFM nanoindentation or microrheology experiments, yield accurate and detailed results on individual droplet but they both face the challenge of sampling highly heterogeneous populations. In the last years, novel microfluidic approaches have been developed. The throughput of such techniques pass the previous once by several orders of magnitude, allowing to tackle new fundamental challenges in many different fields. However, by focusing on steady-state properties, they remain blind to the complex viscoelastic response of these systems, which in many cases is shown to carry rich and precious information. Here we present a novel technique called Rheofluidics, which combines the high throughput of microfluidics with the versatility of traditional rheological probes. Rheofluidics studies the time-dependent deformation of droplets flowing through microfluidic channels with well-defined shape, designed in order to obtain a prescribed, time-dependent hydrodynamic stress on the droplet surface. For instance, by applying a harmonic stress at a given frequency ω, dynamic viscoelastic moduli G'(ω) and G"(ω) can be extracted as routinely done by commercial rheometers on bulk samples, with a throughput more than 1000 times higher the one typically achieved by standard rheology. As a first proof, we use Rheofluidics to study the mechanics of oil droplets in water, regarded as a model system whose stiffness is uniquely determined by the value of the interfacial tension G

Symposium CS

Colloids and suspensions

Organizers: George Petekides and Valeria Garbin

Tuesday 13:20 Virtual / Track 12 CS29

Signatures of elastoviscous buckling in the dilute rheology of suspensions of flexible rods

Anke Lindner[1], Olivia du Roure[1], David Saintillan[2], and Brato Chakrabarti[3]
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As an elastic rod tumbles in shear flow, it experiences compressive viscous forces that can cause it to buckle and undergo a sequence of morphological transitions with increasing flow strength. We use a combined experimental and numerical approach to elucidate these transitions on the particle level. We then use numerical simulations to uncover the effects of these transitions on the steady shear rheology of a dilute suspension of stiff polymers. Our results agree with classic scalings for Brownian rods in relatively weak flows but depart from them above the buckling threshold. Signatures of elastoviscous buckling include enhanced shear thinning and an increase in the magnitude of normal stress differences. We discuss our findings in the light of past work on rigid rods and non-Brownian filaments and highlight the subtle role of thermal fluctuations in triggering instabilities.

Tuesday 13:40 Virtual / Track 12 CS30

Structural Evolution of Nematic Hard-rod Glass during Start-up of Shear Flow: Revelations by Rheo - Confocal Microscopy

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We have examined the response of a dense suspension of purely repulsive hard-rod particles to start-up shear flow using a combination of rheometry and confocal microscopy. We use micron sized silica rods (L ˜ 4.5 µm, L/D = 10) with spherocylindrical shape that exhibit rich liquid crystalline phase behaviour and is a model system to study ideal hard-rods of moderate aspect ratio (˜5-10) at single particle level. Silica rods were suspended in a refractive index matched 74 wt% DMSO aqueous solution. Fluorescently labeled silica rods were mixed with non-dyed rods in 1:200 ratio to be used as tracers. Stress controlled rheometer was combined with confocal microscope allowing us to track individual particle trajectory in a concentrated suspension during linear and nonlinear rheological measurements. It has been previously demonstrated by experiments and simulations, that dense solution of rod-like colloids exhibit collective end-over-end tumbling, kayaking and wagging of the director before flow-aligning at higher shear rates. Here we find that the dense hard-rod suspension consists of randomly oriented nematic polydomains and exhibits solid-like behaviour. These domains are fully flow-aligned at high shear rates with the resultant system exhibiting glassy dynamics. Performing start-up shear measurements we observe transient stress response with two stress overshoots that indicate a two-step yielding process. This behaviour which is captured for the first time was investigated using confocal microscopy. The first stress peak observed at low strain (~100%) is associated with tube renewal of rods and the second stress peak at very large strains (~5000%) is associated with steady state flow of rods while exhibiting wagging.

Tuesday 14:40 Virtual / Track 12 CS31

Shaping hollow fibers of whey proteins aggregates

Alice Vilotte[1], Hugues Bodiguel[1], Komla Ako[1], Christophe Schmitt[2], Deniz Z. Gunes[2], and Clément de Loubens[1]
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The formation and properties of thermally-induced, acidic-induced gel or gel induced by salt-addition have been widely studied in order to modulate the texture of food products. Sensory properties such as the texture of a food product can also be modulated by adding fibres whose high surface-to-volume ratio contributes to the viscosity of the solution. There are currently different techniques for producing fibres such as electrospinning (Torres-Giner et al., 2007) solution blowing spinning (Khansari et al., 2013) wet spinning, gel spinning, or extrusion. In this talk, we show that whey proteins aggregates can be structured as a gelled fiber thanks to a controlled flow. The flow consists in the co-flow of a suspension of submicrometric WPI aggregates in a solution of calcium chloride. We discuss of the effects of the physicochemical and hydrodynamic conditions leading to the formation of stable fibers of about 100 µm diameter. Moreover, quantification of the structure of the fiber by fluorescence labelling and characterization of the kinetics of the reaction-diffusion mechanisms seems to indicate a hollow internal structure of the fiber who seems to be driven by osmotic pressure difference between the calcium and aggregates phases.

Tuesday 15:00 Virtual / Track 12 CS32

Orientational demixing in anisotropic non-Brownian particle suspensions

Narges Mohammad Mehdipour[1], Naveen Krishna Reddy[2], Roman Shor[3], and Giovanniantonio Natale[3]
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The small Angle Light Scattering (SALS) method is used to determine the flow-induced microstructural changes in polydisperse colloidal suspensions of high aspect ratio particles dispersed in a Newtonian fluid. Data are reported for dilute and semi dilute systems consisting of titanium dioxide (aspect ratio of 2.5) rodlike particles suspended in a Newtonian fluid (87.5 wt. % glycerol and 12.5 wt.% water); for Kaolinite nano clay (aspect ratio of 10) platelet particles suspended in the same matrix. In a rectangular capillary, the time evolution of the Anisotropy Factor (AF) and the average orientation angle (θ) of particles during flow has been probed at various distances from the cuvette wall. Using mixtures of rod and plate-like particles, we produced a bi-disperse colloidal suspension of high aspect ratio particles to examine the effect of shape bidispersity on the suspension microstructural dynamics. The transient values for AF and θ are detected continuously for all suspensions at different Pe numbers and different concentrations which is difficult or impossible to be observed by direct imaging techniques. A spatially changing particle orientation is observed caused by the gradient in shear rate in the capillary flow (from the cuvette centerline to the wall). However, no particle migration was encountered. Experimental results also exhibit a good particle alignment in the flow direction at high Pe numbers (around 10^4) at low deformation and then a breakdown in structure followed by orientational demixing at larger deformations. These experimental findings will provide insights that will be helpful in the prediction of the flow properties of polydisperse colloidal suspensions which are often encountered in many industrial processes.

Tuesday 15:20 Virtual / Track 12 CS33

Rheological Analysis of Nanosilica/HPAM Nanofluid for Enhanced Oil Recovery

Owen Kwan[1], Elnaz Erfanian[1], Milad Kamkar[2], Brij Maini[1], and Uttandaraman Sundararaj[1]
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Polymer nanofluid is one of the most promising materials for enhanced oil recovery (EOR) due to its ability to achieve favorable mobility ratios driven by viscosity alterations. Hence, studying the flow behavior of polymer nanofluids is of utmost importance to fully understand the mechanical response of these hybrid solution systems for designing and evaluating the efficiency of polymer nanofluid. This work aims to examine the rheological properties of two different nanoparticle (NP) additives-slightly hydrophobic AER R816 and hydrophilic AER 300-in aqueous solutions with 500ppm, 1250ppm and 5000ppm partially hydrolyzed polyacrylamide (HPAM). Linear viscoelastic properties of the hybrid solution systems were studied under small amplitude oscillatory shear deformation. As deformation in porous media can be rapid and large, consideration of nonlinear viscoelastic properties is essential. Stress decomposition method and Lissajous-Bowditch curves were used to describe the intercycle and intracycle nonlinear responses of the nanofluids. It was observed that polymer and NP concentrations can significantly affect viscoelastic response of the systems in both linear and nonlinear frameworks. In the case of 500ppm HPAM solution, G' showed a dramatic increase of 4 orders of magnitude upon incorporation of 4wt.% AER R816. The results also suggested that the polymer networks can be initially disrupted by the presence of low concentrations (i.e., 2wt.%) of the NP additive before being strengthened at high concentrations (i.e., 4wt.%) of NPs. Strain sweeps in the nonlinear viscoelastic region showed that the addition of NPs causes the polymeric nanofluid behavior to change from shear thinning to weak strain overshoot. This further confirmed the creation of network structures based on the amount of NPs added. Surface chemistry also played a significant role as solutions with slightly hydrophobic NP AER R816 caused up to 10 times higher G' and G" values compared to those containing equivalent weights of hydrophilic NP AER 300.

Wednesday Morning

Symposium PL

Plenary Lecture

Wednesday 8:10 Virtual / Plenary Lecture PL1

Yielding dynamics of soft glassy materials: stress overshoot, shear banding and avalanches

Sébastien Manneville[1], Thibaut Divoux[1], Catherine Barentin[2], Federico Toschi[3], Mauro Sbragaglia[4], and Roberto Benzi[4]

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Soft glasses encompass a wide class of materials characterized by a microstructure made of a dense, amorphous assembly of deformable particles. Such a jammed microstructure leads to features typical of glassy matter including dynamical arrest, aging, and yield stress behaviour. Beside their fundamental interest, soft glassy materials are key to a number of everyday-life applications ranging from foodstuff to cosmetics and pharmaceutical products. When submitted to an external shear, they display a complex solid-to-liquid transition that generically involves a short-time elastic response followed by a stress overshoot and plastic flow. Heterogeneous flows with wall slip and/or shear bands are also ubiquitously reported during the shear-induced fluidization of soft glasses.

In this talk I will first review the phenomenology of shear start-up in soft glasses such as microgels and emulsions, as well as the modelling of their yielding dynamics. I will then recall our seminal experiments on carbopol microgels, which revealed the existence of transient shear banding in soft glassy materials [1]. I will show that a continuum theoretical approach based on a nonlocal fluidity model allows us to accurately reproduce most of the features observed experimentally during shear start-up [2]. Finally I will broaden the discussion to other soft glassy systems and to generalizations of the model that account for steady-state shear banding, avalanche-like behaviour, and brittle-like response.

[1] Divoux et al., Phys. Rev. Lett. 104, 208301 (2010). [2] Benzi et al., Phys. Rev. Lett. 123, 248001 (2019).

Symposium CS

Colloids and suspensions

Organizers: George Petekides and Valeria Garbin

Wednesday 9:20 Virtual / Track 1 CS6

Shear thickening in repulsive and weakly attractive colloidal suspensions

Rathee Vikram, Alessandro Monti, Marco E. Rosti, and Amy Q. Shen

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The onset stress for shear thickening in dense suspensions is determined by the repulsive forces between particles. We control the inter-particle forces in charge stabilized silica colloids by adding a monovalent salt (sodium chloride, NaCl) with different concentrations. We perform systematic rheological measurements by varying the particle volume fractions (0.40-0.55) of spherical silica particles (diameter ~ 420 nm) and the salt concentrations (0-0.5 M). For particle volume fractions ranging from 0.4 to 0.55, at low NaCl concentrations (< 0.3 M), the onset stress decreases exponentially with the salt concentration. At NaCl concentration of 0.3 M, the interaction potential turns attractive, forming small particle aggregates, which results in enhanced shear thinning below the onset stress, followed by reduced shear thickening. In particular, at volume fractions range of 0.45-0.5, the shear thickening behavior can be captured by two varying exponents. At relatively high NaCl concentration (0.4 M), for volume fraction range of 0.45-0.5, the suspension forms percolating particle network, resulting in time and history dependent shear thickening behavior. Supported by simulation studies, we show that this time dependent shear thickening behavior is caused by competition between break and reforming of shear-induced particle clusters and shear-activated frictional contacts. This interplay of cluster formation leads to thinning-thickening-thinning-thickening behavior. By plotting the plateau shear viscosity below onset stress, we also demonstrate that the jamming volume fraction decreases with increasing salt concentration for suspensions without frictional contacts

Wednesday 9:40 Virtual / Track 1 CS7

Migration in dense suspension flows

Ryohei Seto[1] and Masao Doi[2]
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The importance of solid-particle mechanics controlling transport phenomena of dense suspensions has been recognized more and more. Particle simulations for rheological tests have played a pivotal role in revealing such microscale physics. In rheology, we impose uniform-flow conditions to relate stress to deformation-such characterizations should be useful in the fluid mechanical models. However, such uniform-flow characterizations may hide some properties of dense suspensions. Particle migration is one of such vital features in suspension flows. To investigate migration, we extended the particle simulation, LF-DEM, designed to simulate shear-thickening rheology, to general flow conditions. Our new simulation introduces a coarse-grained flow field interacting with the particle phase with the incompressibility condition. It allows us to investigate suspension flows in channel flows and wide-gap Couette devices. We show how the migration besides the contact mechanics affects the transport phenomena.

Wednesday 10:00 Virtual / Track 1 CS8

Experimental evidence of the direct link between inter-particle force profiles and bulk rheology in dense suspensions by tuning-fork AFM

Anh Vu Nguyen Le[1], Guillaume Ovarlez[2], and Annie Colin[1]
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Dense suspensions are soft-matter systems that might display not-fully-understood and complex flow behaviors (e.g. shear thickening, shear thinning, yield stress). The microscopic interactions between the particles - especially pairwise frictional forces - can play a decisive role in explaining the bulk rheology of suspensions at high particle volume fraction. By taking advantage of state-of-the-art techniques of tuning-fork AFM, we evidence the link between the microscopic friction coefficient of the particles and the jamming fraction of the bulk. We mesure the pairwise force profile of polystyrene particles (of diameter ranging from 40 μm to 500 μm), immersed in air and various Newtonian fluids (NaI aqueous solution, silicone oil, and PEG). We find that their coefficient of friction varies with the matrix fluid. The correlation between particles' friction and suspension's jamming fraction agrees with the numerical results of Chèvremont et al. [1]. Furthermore, our results show that friction coefficient decreases with an increasing normal load, following the model from Lobry et al. [2]. Our works help to evidence the impact of particulate friction on the behavior of dense suspensions, which in industries are notoriously hard to process.

[1] W. Chèvremont et al. (2019), Phys. Rev. Fluids, vol. 4, 064302. [2] L. Lobry et al. (2019), J. Fluid Mech., vol. 860, pp. 682-710.

Wednesday 11:00 Virtual / Track 1 CS9

Effect of counter-ions on the rheological properties of mixed surfactant solutions

Zlatina Mitrinova, Hristo Alexandrov, Slavka Tcholakova, and Nikolai Denkov
Department of Chemical and Pharmaceutical Engineering, Faculty of Chemistry and Pharmacy, Sofia university, Sofia 1164, Bulgaria

The ionic surfactant solutions are affected by electrolyte content which changes micelles packing parameter. Such systems rheology is described via "salt curves" with the highest viscosity at intermediate salt concentration. For a single surfactant, more hydrated counter-ions shift the salt curves to higher electrolyte content because they are less effective in screening the electrostatic interactions between the surfactant head-groups [1]. There is no systematic study for the effect of multivalent counter-ions on the rheological behaviour of surfactant mixtures. Here we study the effect of charge, Z, and hydrated radius, R, of cations on the mixed anionic SLES and zwitterionic CAPB surfactant solutions viscosity. The salt curve position goes leftward in the order sodium<potassium<magnesium<calcium<aluminium which confirms the studies with single surfactant [1]. We found that the viscosity at the salt curve maximum decreases when R increases and the salt curve amplitude is higher for potassium compared to sodium, contrary to Pleins et al., [1]. This is probably due to the interplay between the anionic and zwitterionic surfactants, and the electrolyte. The latter effect of the R was confirmed also with the bivalent ions for which the addition of magnesium with larger R than calcium, leads to lower viscosity peak. The governing factor for controlling the position of the viscosity maximum appears to be the ratio between the counter-ion charge and size, Z/R. The higher Z/R ratio leads to lower required amount of electrolyte to reach the viscosity peak.

[1] Pleines, M., et al., *J Colloid Interface Sci* 537, 2019, 682-693.

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Wednesday 11:20 Virtual / Track 1 CS10

Dynamic arrest and confinement effects in symmetric star-linear polymer mixtures

Daniele Parisi[1], Domenico Truzzolillo[2], Vishnu D. Deepak[3], Mario Gauthier[3], and Dimitris Vlassopoulos[1]
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When non-adsorbing linear polymer chains are added to suspensions of multiarm star polymers, the osmotic effects (deswelling and depletion) dictate the resulting rheology. Here we examine the behaviour of linear-star mixtures having the same hydrodynamic size, and show that they exhibit rich dynamics depending on the initial concentration regime of the stars. Linear viscoelasticity was used to investigate the rheological properties of such systems at two concentration regimes for the stars: i) below their overlapping concentration c*, where stars display a liquid-like response and ii) well above c*, where stars show a glassy behavior. In the former case, the presence of an entangled linear chain matrix promotes the formation of arrested states. Remarkably, a progressiver increase of linear polymer chains drives a re-entrant liquid, as a result of an osmotic compression of the star polymers. In the latter case, two distinct scaling regimes are observed for both plateau modulus Gp, and linear polymer matrix relaxation time τ: at low linear polymer concentrations, a weak concentration dependence of both Gp and τ is observed and chains are confined between particles. On the other hand, at higher linear polymer concentrations, the scaling-law for entangled linear polymer chains is recovered, as star polymers are now fully compressed and behave as solid nanofillers. Simple scaling arguments show that the threshold crossover concentration between the two linear polymer concentration regimes corresponds to the maximum osmotic star compression and marks the transition from confined to bulk dynamics

Wednesday 11:40 Virtual / Track 1 CS11

Thixotropy and strain stiffening of aqueous carbon black suspensions

Elie N'gouamba[1], Julie Goyon[1], Thomas Oerther[2], and Philippe Coussot[1]
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Despite the hydrophobicity of carbon black (CB) particles, homogeneous aqueous suspensions of CB can be prepared by dispersing gum arabic in the mixture. These suspensions first appear to be thixotropy fluids: they exhibit a yield stress increasing with the time of rest, their apparent viscosity decreases under shear, and a viscosity bifurcation is observed around the yield stress, the fluid evolving either towards stoppage or to a steady flow at a large shear rate for a small stress change [1]. We checked the validity of these steady flow properties by MRI-rheometry measurements. We then focus on the behavior in the solid regime and remark an original effect. We follow the structural state of the material by measuring its apparent elastic modulus at small deformation during a creep test under various stresses. In contrast with various other yield stress fluids which exhibit a constant elastic modulus in the solid regime [2], the elastic modulus under small deformation of CB suspensions appear to widely increase (up to factor 10) as the deformation is increased up to yielding [1]. This strain stiffening effect finds its origin in the specificities of the (van der Waals) interactions and structure (aggregates) of the particles: the deformation allows more contact points between the particle surfaces, which stiffens the whole material structure.

[1] E N'gouamba, J. Goyon, L. Tocquer, T. Oerther, and P. Coussot.Yielding, thixotropy and strain stiffening of aqueous carbon black suspensions. Journal of Rheology, 64:955, 2020. 97. [2] E. N'gouamba, J. Goyon, P. Coussot, Elastoplastic behavior of yield stress fluids, Phys. Rev. Fluids,4, 123301 (2019)

Symposium PM

Polymer melts and composites

Organizers: Maria Teresa Cidade and Juan de Vicente

Wednesday 9:20 Virtual / Track 2 PM6

Quantification of long-chain branches in essentially linear polyethylenes by analyzing thermorheological complexity

Florian J. Stadler[1], Enrico Troisi[2], Wei Wang[3], Chuangbi Chen[1], Nicolaas Friederichs[2], Rajesh Chitta[2], and Wilma Limpens-Bakker[2]
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Catalytically synthesized polyethylenes (PE), especially metallocene catalyzed polyethylenes (mPE), are known to have rather low long-chain branching (LCB) levels, which is difficult to quantify by classical analytical means. For this reason, a method was derived to utilize the thermorheological complexity induced by sparse long-chain branching to quantify the LCB-level. In the first step the activation energy spectra of phase angle δ(ω) and storage modulus G'(ω) are determined from measurements at 5 temperatures. Several characteristic points from these spectra are then used to determine the type of polymer topography (sparsely branched, tree-like branched, comb-like branched) and get an estimate of the molar mass distribution of the material as well as to check for the reliability of the obtained data by confirming several empirical relations, e.g.

whether the amount of thermorheological complexity with respect to δ is in accordance with the characteristic phase angle δ_{max}, the thermorheological complexity derived equivalent of the characteristic phase angle δ_c. Next, the molar mass M_w is determined from the crossover frequency ω_c, which is possible for materials with narrow molar mass distribution and $\delta_{max}>50°$. As the last step, the branching frequency λ [LCB/1000 C] is determined from M_w and d_{max}. This procedure has been implemented into an automated Matlab script. With this method, it is possible to obtain a whole host of information using rheological standard measurements, for which previously more difficult rheological techniques and expensive analytical techniques like gel-permeation chromatography with coupled light scattering were necessary.

Wednesday 9:40 Virtual / Track 2 PM7

Hydrogel scaffolds: Rheological and microstructural characterization of hybrid structures based on chitosan and collagen

Victor M. Perez-Puyana[1], Mercedes Jiménez-Rosado[1], José Fernando Rubio-Valle[2], Antonio Guerrero[1], and Alberto Romero[1]
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The development of materials as potential scaffolds for tissue engineering is not an easy task. Scaffolds must fulfill specific requirements such as biocompatibility, external geometry, microstructure or enough mechanical integrity. For this reason, tissue engineering is a multidisciplinary field that requires knowledge in chemistry, materials science and biology in order to analyze the different aspects to be considered. By rheological measurements, some critical parameters can be evaluated such as the critical strain, the stability of the scaffolds over time and the evolution of the structure with the combined effect of stress and temperature. In this study, the optimization of the fabrication process for chitosan/collagen-based hydrogels is carried out. Furthermore, a comparison of the properties of chitosan/collagen hydrogels with different polymer ratio is performed. The fabrication process is similar in both cases. During the optimization of the process, the mixing time and gelation temperature and time are evaluated in order to analyze their influence on the properties of the hydrogels. Rheological (time, temperature, frequency, deformation and flow ramp tests), microstructural and biological characterizations have been performed in order to analyze and compare the properties of the different systems produced. Results showed that the incorporation of chitosan gives hydrogels greater thermal and mechanical stability, being higher viscosity and elastic modulus. The microstructural evaluation of the systems revealed an organized heterogeneous structure. Respect the biological characterization, the preliminary tests showed good cell viability, being higher than 75%.

Wednesday 10:00 Virtual / Track 2 PM8

Effects of dehydration on the mechanical and microscopic characteristics of alginate hydrogels

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The design and the manufacture of new biomaterials are crucial for certain biomedical applications such as tissue engineering. One of the main goals of this field is to control the mechanical properties and microscopic structure of the biomaterial in order to ensure its biocompatibility and reliability. In this sense, the most used materials are hydrogels due to their biocompatibility, high water content and tunable mechanical properties. A hydrogel is defined as a three-dimensional cross-linked polymeric network dispersed in an aqueous medium. At equilibrium hydrogels reach a water content up to 99 vol%. This can be modified afterwards by a dehydration process which leads to an increase in the polymer concentration, as well as an interaction between the polymeric chains due to the shrinkage of the material. Thus, this entails a rearrangement of the polymeric network which modifies the microscopic structure and mechanical properties of the dehydrated hydrogel. For these reasons, we compare different dehydration methods for alginate based hydrogels, which allow us to control their microstructure and mechanical behavior. The proposed methods are based on the application of a certain tensile or compressive stress [1,2], which allows to control the dehydration dynamic. We analyzed the effects of the water loss and the applied stress on the fibers rearrangement and mechanical properties. We mechanically characterized the hydrogels studying their Young modulus under static uniaxial tensile tests and their viscoelastic moduli under oscillatory shear tests. These parameters were greatly affected by the degree of water loss and the type of stress applied during their dehydration. The obtained results show the consequences that the water loss and the rearrangement of the polymeric network into anisotropic structures have on the rheological properties of hydrogels.

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Wednesday 11:00 Virtual / Track 2 PM9

Assessing photocuring process of novel PANI/ACRYLIC composites for 3D printing by photorheology: Influence of the photoinitiator agent and PANI amount

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Digital light processing (DLP) 3D printing based on a photopolymer has become a powerful tool to rapidly fabricate 3D objects with an unique shape, high spatial resolution and desired performance. Likewise, the use of 3D printing technologies in electronics has great potential since it allows the integration of sensors, conductors, devices with different electronic functions. However, there is low availability of suitable materials with specific properties, for instance electrical conductivity, to be used in DLP printing. To achieve this goal, it is important to design new photosensitive resins with a conductive filler. In this sense polyanilines (PANIs) are increasing their popularity owing to their electrical behaviour, good environmental stability, simple synthesis and low cost. The main goal of this work is the development of a conductive resin where PANI-HCL was incorporated as a conductive filler into an in-house formulation compounded by Ethyleneglycolphenylether acrylate (EGPEA) as principal monomer, 1, 6-hexanediol diacrylate (HDODA) as a crosslinker, and Diphenyl (2,4,6-tri- methylbenzoyl) phosphine oxide (TPO) serving as photoinitiator. In this formulation the amounts of PANI and photoinitiator were adjusted in order to obtain the best formulation for 3D printing sensor or electronic devices with applications in enery conversion or energy storage. To characterize the photopolymerization process and the network formation, the kinetics of the polymerization was studied in situ using photorheology. Time-sweep measurements were carried out for each formulation and the effect of PANI and TPO concentration in the new composites was studied. Additionally, morphological and cure depth tests were used to support the results. The best formulation was printed by DLP in order to check their processability.

Keywords: 3D printing, electrically conducting polymer, polyaniline, polymer composite, UV curing

Wednesday 11:20 Virtual / Track 2 PM10

Development and characterization of transient double polymer networks with multiscale viscoelastic response

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Polymer gels and networks are fascinating versatile soft materials which are ubiquitous in daily life and high added-value applications. These networks are divided into two categories known as chemical networks and physical networks. Today the biggest challenge is to combine and control within the same material all the distinct features that makes them ideal for application. To address this challenge, a new type of polymer networks, composed of two interpenetrating polymer networks, has been developed with the aim of combining at least two dynamics in the same material, giving rise to multiscale viscoelastic response under external stress or deformation field.

Our objective is to elaborate and study the dynamics of model double polymer networks, only based on supramolecular junctions. In order to obtain the required multiple dynamics, a combination of metal-ligand interactions, phase separation and entanglements is used. The first, short lifetime, network is built from linear polymer bearing terpyridine ligands as side groups and is crosslinked by the addition of transition metal ions. The second, long lifetime, network is made from a phase separated ABA triblock copolymer with a long central block and small outer blocks to ensure strong and stable association.

Here, we first report on the characterization by rheology of the two individual networks derived from these polymers to understand the influence of the tailored bonds in the networks. We show that the properties of the second network strongly depend on the sample composition, and in particular on the length and volume fraction of the outer A blocks of the copolymer. Then, we show that, for the double networks, the viscoelastic response is governed by the interplay between sticker dynamics and chain entanglements. Both processes have a characteristic lifetime, which can be tuned by playing with temperature and/or with the metal ion nature to control the final relaxation of the network.

Wednesday 11:40 Virtual / Track 2 PM11

Elastic long-term behaviour of viscoelastic PVB polymer

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Polyvinyl Butyral (PVB) is a viscoelastic amorphous polymer generally found in composite layered structures such as safety glass or photovoltaic modules. Both structures may experience high temperature loads (e.g., 120-150°C) inside autoclaves during manufacturing or during quality control tests required by international standards. In this regard, current low temperature and short timescale mechanical characterizations might be inadequate to study phenomena such as delamination, de-wetting, and bubble or blister formation-all failure modes shared by both safety glass and photovoltaic modules at high temperatures.

To tackle the above, we pursue an experimental characterization of PVB at high temperatures in shear rheometry using a plate-plate configuration. Relaxation experiments in small deformation reveal that the PVB modulus, at high temperatures and short time scales, is well below presently available long-term elasticity estimates. In current mechanical characterizations, the latter is generally depicted as an extra elastic term in the generalized Maxwell model in the form of G_∞ when in shear. This situation is exacerbated by non-linear effects, in the form of strain softening, at high temperatures. At 140°C, PVB further appears to display time-strain separability. Additionally, we show that the concept of a long-term elasticity might be rendered moot, or in the best-case scenario, it might be linked to a relevant timescale such as the reptation time of the polymer chains. Indeed, we obtain the master curve for PVB at 25°C using frequency sweeps and time-temperature superposition (TTS) and observe that current estimates for G_∞ are correlated with the magnitude of the rubbery plateau. Thus, we can provide time-temperature estimates for the validity of current long-term elasticity measurements while showing how TTS can be used to create a time-temperature phase diagram for PVB delimiting the glass transition, rubbery plateau, and melt states.

Symposium IR

Interfacial rheology, emulsions and foams

Organizers: Anniina Salonen and Nikolai Denkov

Wednesday 9:20 Virtual / Track 3 IR6

Rheology of phospholipid monolayers

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Membrane fluidity of phospholipid bilayers is not only important for compartmentalization of the cytoplasm and organelles in eukaryotic cells but is also crucial for signaling across these membranes. Phospholipid monolayers-one of the bilayers leaflet-have an importance of their own as they coat the alveoli and prevent lung collapse. Therefore, phospholipids are used for pulmonary lung surfactant replacements to prevent lung collapse in premature infants (neonatal respiratory distress syndrome) as well as in adults (acute respiratory distress syndrome). We investigate monolayers of various phospholipids at the water-air and buffer-oil interface. Their linear viscoelastic regime is probed with oscillatory interfacial shear rheology by the interfacial needle stress rheometer (ISR), which is a macroscopic technique. The lipid mixtures under investigation consist of phosphatidylcholines with saturated (palmitoyl) and unsaturated (oleoyl) fatty acids leading to different melting temperatures of the hydrophobic tails. The interactions between the lipids can be tuned by choosing the adjacent bulk phases accordingly, therefore resulting in different phase behavior and rheological properties. A detailed analysis of the mechanical properties of phospholipid monolayers in relevant conditions contributes to a sound understanding of the mechanical properties of phospholipid bilayers.

Wednesday 9:40 Virtual / Track 3 IR7

Flow field-based data analysis for rotating microfabricated probes (the microbutton ISR)

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The coupling between the interfacial and bulk phases flow is inherent to interfacial rheometry. Flow field-based data analysis (FFBDA) techniques [1] directly include the coupling of interfacial and bulk flows even when nonlinear velocity profiles appear at the interface or the subphase and have allowed for precise measurements of interfacial mechanical properties with particularly high resolution in the cases of the magnetic needle and the DWR interfacial rheometers. Another very interesting device is the micro-button interfacial rheometer [2]. A proper consideration of the dynamic coupling between interfacial and bulk phase flows is convenient in order to take full advantage of the high precision of the device. Here we report on a FFBDA scheme developed for the micro-button interfacial rheometer under oscillatory rotational forcing in the two bulk fluid phases configuration. The disparity of length scales in the case of the micro-button - the probe radius is much smaller than the lateral extension of the interface and the depth of the subphase - poses discretization problems and favours non-linear flow velocity profiles. Consequently, we have used a logarithmic discretization in the two spatial coordinates, (r,z), yielding non-uniform meshes with a higher concentration of nodes in the vicinity of the probe rim and the interface. This allows for smaller mesh sizes while assuring good precision in the calculation of the velocity gradients close to the probe's rim. We will show the results of numerical simulations that will illustrate the behavior of the FFBDA code with emphasis on the case of an air upper phase. We will discuss the role of the different characteristic length scales and show that in this configuration the velocity profile at the interface is non-linear in most practical realizations.

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Wednesday 10:00 Virtual / Track 3 IR8

Drag on a spherical particle at the air-liquid interface: Interplay between compressibility, Marangoni flow and surface viscosities

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Particles at interfaces play an important role in a large range of industrial and biological processes. In the majority of these processes the interface is complex, i.e. it exhibits a position- and time- dependent surface tension and/or rheological interfacial stresses, where the latter are possibly deviatoric. Due to the coupling of the interface to the bulk and the intricate interplay between the different physical mechanisms that induce interfacial stress, understanding and predicting the flow dynamics of a particle translating at an interface is not trivial. We numerically investigate the dynamics of a spherical particle embedded symmetrically in a planar air-liquid interface. The interface is assumed to remain planar, and the particle translates tangentially to the interface. Moreover, the interface is endowed with a concentration-dependent surface tension and viscous stresses are added using the Boussinesq-Scriven model. The finite element method is employed to solve the fully coupled set of flow- and transport-equations. We first perform a thorough analysis of the role of mesh- and domain-size for an incompressible interface. We then systematically investigate the role of a non-uniform interfacial tension and interfacial viscosities, paying special attention to interfacial compressibility. For inviscid interfaces, the motion of the particle induces a gradient in surface concentration, which in turn drives a Marangoni flow in the opposite direction, increasing the drag on particle. Our numerical method allows simulations for a large range of Marangoni and Péclet numbers, and we show how these can induce incompressiblity of the interface. We then investigate the role of interfacial shear- and dilatational viscosities, and show how incompressibility of the interface can also be introduced by a large dilatational viscosity. Finally, we systematically investigate cross effects where both Marangoni stresses and interfacial viscosities play a role, and we elucidate their intricate coupling.

Wednesday 11:00 Virtual / Track 3 IR9

Interfacial shear rheology of polyelectrolyte microgels confined to oil-water interfaces

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Numerous industrial applications require precise control over the stability of emulsions and foams. The use of smart emulsifying agents such as stimuli-sensitive microgels allows for on-demand inversion or breaking of the system by mild changes in external conditions [1,2]. Microgels, three-dimensional, cross-linked polymer networks, are soft colloidal objects swollen by the solvent [3]. Owing to their softness, they behave fundamentally different under interfacial confinement as compared to rigid particles. Their behavior at fluid interfaces and, thus, emulsion stability does not only depend on the interfacial tension but also on the viscoelastic properties of the microgel-laden interface involving swelling, interpenetration, elasticity, and deformability of the networks [4,5]. Using a double wall-ring geometry combined with a Langmuir trough, we probe the mechanical response of monolayers of polyelectrolyte microgels adsorbed to decane-water interfaces while simultaneously controlling the surface pressure, i.e., the microgel interfacial concentration. We correlate the rheological properties of the monolayer with the two-dimensional phase behavior of the microgels which is associated with an isostructural phase transition between a non-close-packed and close-packed arrangement. Before phase transition, moduli values increase with increasing surface pressure and the linear viscoelastic regime extends to higher strain. In addition, monolayers of charged microgels generally yield higher elastic response than monolayers of uncharged microgels (at the same surface pressure). During phase transition, the moduli values decrease but re-establish once phase transition is completed.

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Wednesday 11:20 Virtual / Track 3 IR10

Adsorption kinetics and interfacial shear rheology of whey protein isolate at oil/water interface

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In this study, the adsorption behaviour and interfacial shear rheological properties of whey protein isolate (WPI) at sunflower oil/water (o/w) interfaces was characterized using a pendant drop tensiometer and a rheometer equipped with a Du Nöuy ring geometry. The impacts of bulk protein concentration Cp, pH (3 and 7) and heat treatment (unheated and 90 °C for 30 minutes) were studied by monitoring changes in the interfacial pressure and mechanical properties of WPI adsorbed interfaces. Increasing Cp facilitated faster migration and unfolding of whey proteins at the o/w interface. The elasticity of WPI stabilized interfaces increased with Cp (<0.1 wt%). A further increase in Cp (to 1 wt%) led to reduction in mechanical strength of the interfacial films due to monolayer collapse and formation of multilayers. The rates of diffusion and unfolding of WPI were faster at pH 3 than pH 7. However, the shear moduli of interfacial film were lower at acidic pH which was indicative of a weaker film. Heat treated whey proteins became more surface active with faster diffusion rate and greater equilibrium interfacial pressure than unheated proteins. The elasticity of the interfacial films formed by heated WPI was higher. The extent of heat-enhanced interfacial activity was greater at pH 7 than pH 3, which may be associated with more extensive increases in surface hydrophobicity and protein flexibility under neutral pH. The environmental and processing conditions have considerable effects on the interfacial properties of WPI at the o/w interface. The combination of interfacial pressure and shear rheology measurements provided comprehensive information on the surface activity of whey proteins, the development of interactions between adsorbed WPI molecules and ensuing mechanical properties of interfaces under different solvent conditions. Such knowledge can contribute to design structured products with improved quality and to better understand the stability of dairy emulsions during subsequent processing, digestion or storage.

Wednesday 11:40 Virtual / Track 3 IR11

Self-assembly of polyelectrolytes membrane

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A variety of industrial and biological processes revolve around complicated physics of fluid-fluid interfaces. Such systems include biological cells, emulsions, bijels, capsules and so on. The mechanical properties of a fluid-fluid interface are of the upmost importance for its stability. A possible approach to stabilise an interface is by forming a complex via dissolving two interacting (poly)ionic species in different immiscible phases. Upon the contact polycations and polyanions will spontaneously diffuse towards the interface and form a membrane or a coacervate through non-covalent interactions. The rheology and the mechanics of complex interfaces were studied extensively in the past years. However, the lack of detailed experimental observations on the mesoscopic level hinders the understanding of the self-assembling membranes growth kinetics. The aim of our work is to link the kinetics of the membrane growth and its morphology on the molecular level to the macroscopic observations of its rheological properties. In our study, chitosan, a water soluble cationic polymer, forms a complex with oil soluble anionic phosphatidic acids at a water/oil interface. We study the interfacial rheometry of the forming film in order to relate the evolution of its mechanical properties to the reaction time and thickness of the membrane. We find that interfacial shear moduli of the interface increase rapidly in a short term and continue to grow linearly in a long term, governed by a simple diffusion. We deploy confocal microscopy and scanning electron microscopy (SEM) in order to understand the morphology of the membrane. We discovered an inhomogeneous, patch-like structure of ultra-thin films (100 nm) and droplet inclusions in the thick films (10 μm). The dynamic lightscattering (DLS) of the forming film showed us that while the complexation between chitosan and phosphatidic acids starts virtually instantaneously the interface formation is a non-uniform process both morphologically and kinetically.

Symposium MS

Modelling and simulations

Organizers: Natalie Germann and Daniel Read

Wednesday 9:20 Virtual / Track 4 MS6

High Weissenberg number simulations with incompressible Smoothed Particle Hydrodynamics and the log-conformation formulation

Jack King and Steven Lind

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Viscoelastic flows occur widely, and numerical simulations of them are important for a range of industrial applications. Simulations of viscoelastic flows are more challenging than their Newtonian counterparts due to the presence of exponential gradients in polymeric stress fields, which can lead to catastrophic instabilities if not carefully handled. A key development to overcome this issue is the log-conformation formulation, which has been applied to a range of numerical methods, but not previously applied to Smoothed Particle Hydrodynamics (SPH). Here we present a 2D incompressible SPH algorithm for viscoelastic flows which, for the first time, incorporates a log-conformation formulation with an elasto-viscous stress splitting (EVSS) technique. The resulting scheme enables simulations of flows at high Weissenberg numbers (accurate up to Wi=16 for Poiseuille flow). The method is robust, and able to handle both internal and free-surface flows, and a range of linear and non-linear constitutive models. Several test cases are considered, included flow past a periodic array of cylinders and jet buckling. This presents a significant step change in capabilties compared to previous SPH algorithms for viscoelastic flows, and has the potential to simulate a wide range of new and challenging applications.

Wednesday 9:40 Virtual / Track 4 MS7

Mimicking the rheological properties of polymer solutions using Smooth Dissipative Particle Dynamics

David Nieto Simavilla and Marco Ellero

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The macroscopic simulation of complex manufacturing flows involving viscoelastic fluids remains a challenge due to the complex and computationally expensive modeling required to mimic real rheological behavior. To bridge the gap between molecular and macroscopic levels of description, we propose a bottom-up mesoscopic model to reproduce the viscoelastic behavior of polymer solutions without the need to resort to approximate constitutive equations. We employ Smooth Dissipative Particle Dynamics (SDPD) - a GENERIC compliant Lagrangian discretization of Navier-Stokes equations with thermal fluctuations - to mimic their behavior under dilute and semi-dilute conditions. In this model viscoelasticity is introduced by forming chains of SDPD particles linked by FENE springs. In a first application of the model, we subject these mesoscopic solutions to standard Couette and reverse Poiseuille flow and characterize their rheology (non-Newtonian viscosity, normal stress coefficients and relaxation dynamics) over a wide range of Weissenberg numbers and relative concentrations. Our simulations show the importance of tuning the balance between hydrodynamic and elastic forces to reproduce the correct transition between the different concentration regimes in polymer physics: dilute, semi-dilute unentangled and entangled. In a second application of our model, we simulate the flow around a periodic array of cylinders confined in a channel and study the transition between viscous and inertia-dominated drag for these mesoscopic fluids. Results from both applications show that the modeling of polymeric solutions at the mesoscopic scale is useful tool towards the realistic simulation of complex macroscopic polymeric flows.

Wednesday 10:00 Virtual / Track 4 MS8

The closed form Adaptive Length Scale model in simple and complex flows

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In this paper we employ the closed form of the Adaptive Length Scale (ALS-C) model[1] and investigate its characteristics and potential use in numerical studies of dilute polymer solutions in general flows. The derivation of the ALS-C model was originally inspired by the ability of a Kramers chain to capture important properties of dilute polymer solutions in rapidly varying extensional flows, such as coil-stretch hysteresis.The model introduces two variable extensibility parameters which adapt to the flow changes that modify the developed stresses. The ALS-C can be considered as a generalised version of the Finitely Extensible Nonlinear Elastic model that follows the Peterlin approximation (FENE-P). In proposing the model it was hoped that it would be capable of predicting the enhanced pressure drop observed in many flows of dilute polymeric solutions, but this hypothesis has never been tested in complex flows.

The ALS-C model has not been yet considered in flows outside of simple homogeneous shear or extension and specifically not in any general computational fluid dynamics (CFD) simulations. The model has been implemented into an in-house CFD solver appropriate for viscoelastic fluids[2], while for enhanced stability the log-conformation approach[3] is employed within a finite-volume methodology. Here, we demonstrate the set of equations that need to be solved together with a modified approach that enhances the computational speed for evaluating the instantaneous changes in the adaptive length scale as a result of the instantaneous changes in the flow field. Initially, the performance of the model is illustrated for standard rheological and steady-state shear flows. Finally, its performance in flows within a range of complex geometries is presented, with particular emphasis placed on the estimation of the pressure drop and comparison with experimental data.

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Wednesday 11:00 Virtual / Track 4 MS9

Effect of non-Gaussian end-to-end distributions on shear and elastic gel moduli: theoretical and experimental approach

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Despite its huge potentiality, main limitations of the ideal rubberlike elasticity theory reside in the impossibility to account for polymer chain stiffness, high-order interchain bonding terms and a non-Gaussian distribution of polymer segments, reflecting into a non-Gaussian end-to-end length statistics [1]. Especially this last aspect can play a very important role as hydrogels synthesized by bimodal chain length distributions give rise to networks [2] whose features cannot be modeled by classical rubberlike elasticity theory. Aim of this work was thus to reformulate a rubberlike elasticity theory by considering three non-Gaussian end-to-end length statistics and recalculate shear (G) and elastic (E) moduli dependencies on swelling degree and extension ratio. Particularly, attention was on achieving the configuration integral and the so-called perfect gas term at variable functionality upon Laplace, Cauchy and continuous Poisson (in exponential limit) laws, as they have the two-fold aim to formally mimic the Gaussian law but quantitatively deviate from it to a non-perturbative extent. Interestingly, despite the formal complexity coming from the statistical mechanics treatment, final equations for G and E, whatever the distribution regarded, are reasonably simple and suit to a prompt comparison with available gel data. To infer the most likely end-to-end length distribution in an arbitrary network, a theoretical-experimental approach based on LF-NMR was devised. Application of this strategy to agar 1 %, alginate 1 % and scleroglucan 2 % hydrogels (wt %) reveals that the end-to-end distribution should be never deemed as Gaussian even if, as in agar and scleroglucan systems, the normal statistics is the best among those here regarded. Remarkably, Poisson law is proved instead to be the most realistic for alginate hydrogels.

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Wednesday 11:20 Virtual / Track 4 MS10

Fluctuations in viscoelastic liquids: Development of a general framework

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Dissipation is always accompanied by fluctuations as stated by the fluctuation-dissipation theorem, a key result of nonequilibrium statistical mechanics. Correspondingly, also viscoelastic liquids contain fluctuations, which are relevant particularly for the behavior on small scales, e.g., in microrheology and filament break-up.

To date, models for complex fluids do not address fluctuations systematically. In our recent work, we have extended conformation-tensor based models for polymer liquids by including thermal fluctuations in a thermodynamically consistent way [1] and studied the behavior under deformation [2]. This modelling approach is complemented by establishing the link between the fluctuating conformation-tensor model and the underlying description of polymer chains as bead-spring dumbbells [3]. It is shown that, if the number N of dumbbells is finite, the conventional form of the entropy for the conformation tensor $\mathbf{c}$ needs a finite-size correction, which is derived by statistical mechanics. Furthermore, the explicit form of the fluctuations on $\mathbf{c}$ is established, incl. the N-dependence.

For modeling fluctuating viscoelasticity, we advocate using the square root of the conformation tensor, rather than the conformation tensor itself [1]. While the square root is not unique, we present a procedure for fixing a specific gauge [4]. It is to be noted that modeling in terms of the square root is also useful in the absence of fluctuations, in order to substantially delay the onset of numerical flow-instabilities (e.g. flow around a cylinder) [5].

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Wednesday 11:40 Virtual / Track 4 MS11

A theory for the inhomogeneous flow of chemically-responsive polymer solutions

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Chemically-responsive polymers are macromolecules that respond to local changes of chemical composition of the solution by changing their conformation. The conformation change can occur in response to a change in pH or salt concentration and can lead to drastic changes of the radius of gyration of polymers, with a remarkable example being the transition from a coil conformation to a globule state. Such conformation changes have a strong impact on the viscoelastic properties of the suspension. Typically, the mechanical response of a mixture of polymers and solute is investigated in rheometric flows whereby the shear rate is homogeneous, the flow is unidirectional, and the concentration of polymers and of solutes are constant in space. However, in many situations these quantities change in space, as in the case of Poiseuille flow or flow past obstacles, resulting in inhomogeneous rheological properties of the suspension. In this paper, we present a theory for the flow of a mixture of a solute and of chemically-responsive polymers, which is valid for flows with curved streamlines and inhomogeneous concentration of polymers and of solutes. To model the polymer conformation changes introduced by the interactions with the solute molecules, we consider the polymers as linear elastic dumbbells that respond to changes of the solute concentration by changing the stiffness of their spring. To derive the equations governing the evolution of the variables, we use the Onsager's variational principle, which unveils novel couplings between the distribution of dumbbells and of the solute. Using a linear stability analysis, we show that the governing equations predict an equilibrium and a shear-induced phase separation whereby a homogeneous distribution of solute and dumbbells spontaneously unmix. Similar phase transitions have been observed in previous experiments using stimuli-responsive polymers.

Symposium FB

Food and bio-rheology

Organizers: Jan Engmann and Clément de Loubens

Wednesday 9:20 Virtual / Track 5 FB6

Coagulation characteristics of the heparinized whole human blood neutralized by UHRA and protamine

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Heparin is commonly used to provide anticoagulation of the blood during surgeries; however, bleeding is one of the adverse side-effects of heparin usage. Although protamine can be administered to neutralize heparin and is the only clinically available heparin antidote, protamine does come with severe limitations and its side-effects. The objective of the current study is to utilize small amplitude oscillatory shear (SAOS) rheometry to investigate the dynamics and the qualities of blood clot formation upon heparin neutralization using two different heparin antidotes. Different concentrations of protamine and the newly developed universal heparin reversal agent (UHRA-7) were applied to heparinized whole human blood under three different oscillatory frequencies, two of which were mimicking physiological heart rates. The blood clot formed upon heparin neutralization was analyzed using several key rheological parameters and the use of scanning electron microscopy (SEM), which visualized the morphology and microstructure of the blood clot after heparin neutralization and provided measurements on fibrin fibre to support the rheological observations. It was found that the blood clot structure had significant differences between the clot formed under an oscillatory frequency that mimicked the physiological heart rate and a lower oscillatory frequency commonly used in current clinical measurements. Protamine's limited working dose range and its intrinsic anticoagulation behaviour were observed during the current study; whereas, UHRA-7 showed a larger heparin neutralization window. By relating the global assessment of rheological parameters and microstructure of the clot, the current study provided a connection between fibrin fibre thickness and SAOS measurement, including storage modulus and blood clot's contractile force, to describe anticoagulant reversal and blood coagulation dynamics. A mechanical characterization based on the rheological data was also conducted to provide a further assessment of blood coagulation.

Wednesday 9:40 Virtual / Track 5 FB7

Blood clot phenotyping by LAOStress

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Fibrin networks show strain hardening, Mullins effect, and nonlinear stress-relaxation. Due to the rich mechanical response, rheometry can provide important information on a blood clot's phenotype. Viscoelastic tests together with treatment protocols based on cut-off values are already used for postoperative patient care, but since now only the linear behavior of clots is tested. Measuring at broader ranges of deformation will add

information because blood flow compels clots into a dynamic non-linear response that also alters clot remodeling. To characterize the influence of platelets on clot behavior, a stress amplitude sweep test (LAOStress) was applied to clots from native plasma. Five platelet concentrations were set out of platelet-rich (PRP) and platelet-poor plasma to gain PRP titers from 4 - 64. Five species were used to validate the protocol (human, cow, pig, rat, horse). The oscillation cycle for each stress level was analyzed by using Lissajous plots: minimum-stress and large stress compliance (J_M', J_L') as well as stress softening ratio (R) were the extracted parameters. Cyclic stress loading generated a characteristic strain response that scaled with the platelet quantity at low stress, and that was independent from the platelet count at high shear stress (> 200 Pa). At low shear stresses platelets augmented clot softening due to network alignment on microscopic scale, whereas beyond a threshold macroscopic stiffening occurred. This general behavior was valid in the animal models except in cow. Here, the specific fibrinogen chemistry induced a stiffer network and a variant high stress response: alignment took place until the clot yielded. The new protocol proposed here provides several thresholds to connect the softening and stiffening behavior of clots from native blood plasma with the applied shear stress, points to the reversible part of deformation (residual strains were mostly removed prior to the reading), and thus opens a new route to describe a blood clot's phenotype.

Wednesday 10:00 Virtual / Track 5 FB8

Effect of rheology of simulated mucus solutions on droplet generation during sneezing

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Aerosol formation and propagation during sneezing is a major contributor to the spreading of contagious diseases. Direct observation of the physical mechanism of droplet formation during sneezing via high speed videography of human subjects has revealed that droplet generation follows a complex sequence of events, whereby the expelled mucus volume is flattened into a sheet that expands and thins over time [1]. This is accompanied by the appearance of holes and thin filaments within the sheet, which subsequently destabilize and break up into droplets [1]. The viscoelastic character of the dissolved mucins in sneeze ejecta has a strong effect on the dynamics of filament stretching, which retards the onset of droplet formation and influences droplet size. The process of aerosol generation during sneezing is systematically replicated using an impinging jet setup, whereby the collision of two liquid jets forms a thin fluid sheet that subsequently fragments into ligaments and droplets [2,3]. Experiments are conducted with artificial mucus substitutes that capture the range of viscosities and elasticities in physiological samples. The viscoelastic mucus substitutes are compared against Newtonian mixtures of glycerol and water. Due to the radial flow profile that is established within the sheet, extensional stresses dominate over shear stresses. We examine the effect of mucin concentration on sheet geometry and droplet generation, focusing on the correlation between extensional stresses and aerosol propagation. We summarize our results in terms of the dimensionless Weber, Reynolds, and Deborah numbers.

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Wednesday 11:00 Virtual / Track 5 FB9

Towards in vivo nano-rheometry measurements during oral food processing

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The mechanism of oral destruction of food while eating may only last a few seconds, yet this short oral processing determines our complete perception of texture, taste and aroma of the product. In order to design future delicious, sustainable and healthy food the process of oral destruction should be investigated more thoroughly. However, previous methods involved either measuring textural changes of food before and after the process, or invasively, where the oral process is likely to be influenced. Therefore, we are developing a non-invasive in vivo method that measures textural changes without affecting the oral process.

To determine the rheological properties of food in vivo we use magnetic nanoparticles (MNP) and AC susceptometry (ACS). The magnetic relaxation process of the used MNP systems is dominated by Brownian relaxation and provides the (nano-)rheological properties of its suspension medium. ACS remotely measures the dynamic magnetic response of the particles in an externally applied alternating magnetic field and determines the rheological properties of food, e.g. viscoelasticity and texture non-invasively during the entire oral processing.

The ACS setup consists of an excitation coil and differentially coupled detection coils in a concentric configuration that together with electronics measures the in-phase and out-of-phase components of AC susceptibility in a frequency range of 10-1000 Hz. A temperature-controlled water bath with a water-jacked beaker is used. As a proof-of-concept the in vitro melting of a tomato gel consisting of tomato puree with 1.6 wt.% gelatine and 5 wt.% MNPs with a mean particle size of 100 nm is studied. ACS of the tomato gel at a range of 20-50°C is measured and a viscoelastic ACS model is used to extract the frequency dependent shear modulus and viscosity. The estimated values are then compared with common oscillatory rheological measurements under the same conditions which highlights the advantages and the disadvantages of the nano-rheological technique.

Wednesday 11:20 Virtual / Track 5 FB10

Bolus rheology of texture-modified foods

Mats Stading
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Healthy individuals apply unconscious, but well-coordinated strategies for oral processing producing easy-to-swallow boluses. However, for an increasing proportion of the population the actual swallowing causes problems. Swallowing disorders, or dysphagia, affects 40% of the ones older than 70 due to dementia, trauma or medication side effects. Dysphagia management consists of intake of texture-modified foods with texture depending on the severity of the disorder. The food texture is modified according to common practice and guidelines, whereas it is actually the rheological of the bolus of the food ingested that affects safety and ease of swallowing.

Bolus rheology was determined for five healthy subjects for a set of solid foods. The softest class was gel food, then a smooth timbale and these were compared to the corresponding regular food. The foods investigated were bread, cheese, tomato and the combination of these into a sandwich, all for the respected texture class. The subjects chewed until ready to swallow and the bolus was then immediately measured for complex shear modulus and viscosity. Extensional viscosity was determined for the respective food mixed in a saliva buffer to mimic bolus conditions.

The rheological results showed that the intended adjustment of food texture influenced the bolus rheology in the desired way with decreased viscosity and modulus for increased degree of modification. Another effect of the texture modification was that saliva content as well as chews-to-swallow decreased with degree of adjustment. Overall, the bolus saliva content was lower for the combination of the foods (sandwich) than for the individual components. The results also indicate that the body compensates for the varying food moisture content and keeps the bolus saliva content rather constant. All boluses of the texture-modified foods showed a considerable amount of extensional viscosity, which is important for bolus cohesiveness.

Wednesday 11:40 Virtual / Track 5 FB11

Rheology of feces and CFD modeling of rectal evacuation

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Defaecation is the voluntary evacuation of faeces from the rectum. Disorders of defecation occur frequently in the population and can seriously degrade the quality of life. However, the classification of these disorders and the relevance of the current tests for evaluating colonic and anorectal function are subject to ongoing debate as our understanding of the process of defaecation is currently incomplete. From a fluid mechanical point-of-view, defecation consists in the extrusion of a yield stress material through the anal sphincter. In this talk, we will present a rheological characterization of human feces, suspension of barite modeling feces, and a CFD model of rectal evacuation based on real in-vivo recto-anal motility data. The rheological characterization allowed us to evaluate the range of yield stress of feces values, which vary over several orders of magnitude (up to 8 kPa). The CFD model is based on a combination of X-ray videodefecography and lattice-Boltzmann methods for yield stress fluids and moving boundary conditions to calculate the fields of velocity and stresses during defecation. Simulations revealed that the viscosity of the constitutive Bingham law has a minor influence on energy dissipation during defecation, whereas this dissipation increased linearly with the yield stress. Moreover, the energy dissipation is mainly located at the wall of the anal junction, meaning that this junction is the main resistance to defecation. In conclusion, the rheological characterization of feces and the CFD model shows clearly that yield stress is a major parameter that can impaired rectal evacuation, and open routes to a better understanding of pathophysiology of defecation. Our model could also be used as a diagnostic model by fixing the standard results of normal defecation.

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Symposium ER

Experimental methods and rheometry

Organizers: Christian Clasen and Mariana Rodriguez Hakim

Wednesday 9:20 Virtual / Track 6 ER6

Rheological behavior of lubricants at low temperatures

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In certain applications such as in transmission units of vehicles or windpower generators lubricants are also used at very low temperatures (down to -70°C). How lubricants must be designed to be effective at low temperatures is still largely unknown. Manufacturers and users are therefore looking for robust rheological measurement protocols allowing for assessment of the low-temperature rheological behavior of lubricants. In this context, the base oil has a major influence on the properties of the grease produced from it. The behavior of the base oil, in turn, is very much determined by its crystallization behavior. Another factor which significantly influences the properties of a grease is the structure of the thickener.

There are several measurement standards according to DIN and ASTM according to which lubricants can be characterized. However, the results of the measurements according to standards are determined only at defined temperatures and are limited to individual cases with defined operating parameters. A thorough rheological characterization of selected base oils covering a wide range of applications is presented here, especially focusing on the temperature range down to -40°C. The measured crystallization temperatures depend largely on the different cooling conditions. Furthermore, model greases including different amounts of metal soap as thickener were prepared from these oils. We could show that the yield stress obtained from rheological measurements nicely correlates to common tribological characteristic values of consistency (penetration depth). The shear viscosities of the lubricants were measured using rotational capillary rheometry (up to 10^6 s^{-1}), both at room temperature and at -20°C. These data reveal the critical shear energy required to break down the structure built by the metal soap. Deeper insight into the structure of the grease was gained employing multi particle tracking microrheology and high-frequency oscillatory squeeze flow.

Wednesday 9:40 Virtual / Track 6 ER8

Simultaneous dielectro/rheological measurements in thermoplastics, rubbers and thermosets materials

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Rheology is, more and more, a technique that can be used coupled with other techniques. For example, Dielectric Analisys. Dielectric Analysis measures the two fundamental electrical characteristics of a material capacitance and conductance as function of time, temperature and frequency. Dielectric analysis is powerful technique for characterizing polar materials (with permanent or induced dipoles) such as most of polymers, foods, pharmaceuticals, etc. There is a broad range of applications where this technique is very valuable like phase separating systems, curing kinetics of materials such as epoxy and urethane systems, polymer blends, and nanocomposites.

Wednesday 11:20 Virtual / Track 6 ER10

Charge transport and glassy dynamics in polymerized ionic liquids

Ciprian Iacob[1], Maxi Hoffmann[1], Matthias Heck[1], Atsushi Matsumoto[2], and Manfred Wilhelm[1]
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Polymerized ionic liquids (PILs) combine the attractive mechanical characteristics of polymers and unique physico-chemical properties of low molecular weight ionic liquids in the same material [1, 2]. PILs have shown remarkable advantages when employed in electrochemical devices such as dye-sensitized solar cells and lithium batteries, among others. Understanding their ionic transport mechanism is the key for designing highly conductive PILs. In the current study, the correlation between morphology and charge transport in a homologous series of PILs with systematic variation of the anions is investigated using rheo-dielectric, differential scanning calorimetry and X-ray scattering [3]. Rheo-dielectric is known to be able to cover 23 to 30 decades in frequency by constructing a master curve. As the volume of the counterions increases, the pedant-to-pedant separation increases, and ionic conductivity consequently decreases. The cations dominate structural dynamics since they are attached to the positively charged polymer chains, while the counterions are smaller and more mobile ionic species thereby controlling the ionic conductivity. Further interpretation of decoupling of ionic conductivity from the segmental relaxation enabled the correlation between polymer morphology and ionic conductivity. This study underscores the need for smaller counterions to obtain polymer electrolytes with higher ionic conductivity and decoupling index.

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Wednesday 11:40 Virtual / Track 6 ER11

Progress and challenges on relating 'nonlinear oddities' in oscillatory shear to structural buildup in nanostructured fluids

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The nonlinear oscillatory shear material response of complex fluids has been shown to exhibit peculiar behavior, i.e. 'nonlinear oddities'. By 'oddities' we refer mainly to (i) non-quadratic scaling of the third relative higher harmonic (I3/1) with the strain amplitude in the medium amplitude oscillatory shear region (MAOS) and (ii) strong dependence on the applied angular frequency in I3/1 and of the viscous third relative Tschebyshev coefficients (v31). We have previously correlated such 'oddities' to percolation in nanostructured fluids. Here we provide an overview of progress and challenges based on our work on polymer based nanocomposites, nanocellulose suspensions and pressure sensitive adhesives. In polymer nanocomposites based on conductive fillers unique nonlinear 'oddities' are recorded for filler concentrations corresponding to the electrical percolation threshold in both I3/1 and v3/1. For supercritical concentrations, the 'oddities' further develop and include I3/1 scaling exponents equal to zero as well as multiple scaling laws (three regions) within MAOS. For a given filler morphology, there appears to be little influence of the molecular topology of the polymer matrix, and the non-linear behaviour could therefore be mainly related to the filler morphology and dispersion levels. In suspensions, (mainly focused on aqueous cellulose nanocrystals (CNC) suspensions), similar 'oddities' can be also observed, however, their relationship to gelation is more challenging to assess (similarly also for adhesives). For aggregating CNC suspensions 'oddities' of type (i) in the form of single and three-scaling regions, and (ii) could be observed. Grafting of surface groups having various topologies can qualitatively mimic the nonlinear behaviour of untreated samples at higher concentrations. In self-assembling CNC suspensions, the nonlinear behaviour appears to correspond to the particular phased investigated, with differences in behaviour especially between biphasic and liquid crystalline phases.

Symposium PM

Polymer melts and composites

Organizers: Maria Teresa Cidade and Juan de Vicente

Wednesday 9:20 Virtual / Track 7 PM34

Alginate ferrogels with huge elongation under magnetic stimuli

Francisco J. Vazquez-Perez, Laura Rodriguez-Arco, Cristina Gila-Vílchez, Juan D. G.Lopez-Duran, and Modesto T. Lopez-Lopez

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In these last years, the field of soft actuators and robotics is attracting attention due to their applications in technological fields such as sensors, grippers or locomotion. While this field is mainly dominated by elastomers, hydrogels are progressively attracting more attention due to their biocompatibility and biodegradability [1]. Moreover, they can respond to different stimuli like temperature, pH or electro-magnetic fields. Among them, the application of external magnetic fields is a common way to obtain interesting effects such as movement or magnetrostriction, which consists of the deformation of a material upon magnetization. In this work, we study the magnetostriction effect of alginate ferrogels prepared by three different methods in order to modify their Young modulus, as this quantity crucially influences the ease of the magnetic particles to move in the polymeric matrix. Moreover, this study was carried out for different concentrations of silica-coated iron magnetic particles as well as an increasing and decreasing intensity cycle of the applied magnetic field [2]. Thus, we perform a complete study on the mechanical and microstructural properties of the different alginate ferrogels and relate them with the observed magnetostriction effect. We also propose a theoretical model which reasonably predicts the magnetostriction effect obtained in our experiments. Finally, we compare our magnetostriction results with those of elastomers [3,4], and we show that using our alginate ferrogels is possible to obtain higher deformations under the same magnetic field intensity.

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Wednesday 9:40 Virtual / Track 7 PM35

Melt rheology as a tool to assess the tuning of the degradation rates of Polycaprolactone and Poly(butylene succinate-co-butylene adipate)-based nanocomposites

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The development of biodegradable polymers for packaging, electronics and agricultural uses would partially solve the problem of plastic waste accumulation. Polycaprolactone, PCL, and poly(butylene succinate-co-butylene adipate), PBSA, are receiving increasing attention for their promising biodegradability. Although their fast degradation might be favourable in some applications it renders them unfavourable in applications requiring durable polymers. Interestingly, the use of additives, such as layered double hydroxides, LDH, has shown to alter the rate of degradation of polymer materials [1]. This leads to encouraging prospects of tuning degradation rates of biodegradable polymers for specific applications. It is known that the melt flow behaviour of polymer composites encompassing LDH particles are dependent on the interaction of the LDH particles with the polymer matrix [2], at the same time, the linear viscoelastic properties in dynamic experiments are sensitive both to the chain scission and to the three-dimensional network formation in the polymer matrices. Thus, melt rheology provides a convenient tool to study the competition of chain scissions and recombination reactions occurring through ageing. Here, we follow the degradation rates of PCL- and PBSA-based nanocomposites with various amounts of LDH loadings through the changes in their viscoelastic behaviour. It is clear from our studies that the presence of LDH enhances the lifetime durability and modulates the degradation rate of the elaborated bio-nano composites, and importantly we demonstrate that the rate of degradation is strongly dependent on the LDH loading.

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Wednesday 10:00 Virtual / Track 7 PM36

Storage factor as new parameter for analysis of reinforcement in polymer nanocomposites

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Polymer nanocomposites exhibit complex rheological behaviour due to physical and possibly also chemical interactions between individual components (polymer, nanofiller, compatibilizer in case of unpolar polymer), which can be detected by rheology. Usually, flow behaviour of multiphase polymer systems has been described by storage flow part through the storage modulus curve (formation of secondary plateau) and by loss flow part through dumping behaviour (e.g. Van Gurp-Palmen-plot, Cole-Cole plot), respectively. On the contrary to typical rheological analysis, new approach using information about storage flow part through rigidity behaviour has been introduced for description of physical network made of solid particles in polymer matrix as relation of $\int G'/\int G''$ over specific frequency range. This approach has been experimentally proved for polymer nanocomposites in order to evaluate both shear as well as elongational flow field. In this contribution, nanocomposites with different polymers and fillers have been compared using novel "cumulative storage factor" parameter. It has been found that information obtained from specific cumulative rheological parameters allows detailed analysis of different effects (e.g. formation of physical network, change in average molar mass) that act simultaneously during processing of nanocomposites and are not possible to evaluate from typical rheological or morphological parameters.

Symposium CF

Complex flows

Organizers: Rossana Pasquino and Francisco Galindo Rosales

Wednesday 11:20 Virtual / Track 7 CF1

Rheology of a dilute suspension of rigid fractal aggregates in shear-thinning fluids

Marco Trofa and Gaetano D'Avino
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Suspensions of solid particles are commonly encountered in several industrial and biological systems, e.g., loaded polymer melts, paints, inks, rubber compound, food, blood, drug delivery. It is well-known that the rheological behaviour of these multiphase materials is strongly affected by the solid concentration, particle shape, and the nature of the suspending fluid. Many theoretical, experimental and numerical works have focused on the bulk rheology of suspensions made of particles with simple shapes (spheres, ellipsoids, infinitely long rods) suspended in Newtonian fluids. In real systems, however, the particulate material generally consists of particles with irregular shape. In addition, the suspending liquid may show a non-Newtonian behaviour. A typical example is in the tyre industry where, during the processing stage, particles of carbon black added to a non-Newtonian fluid (rubber) can agglomerate and form complex structures. In this contribution, we investigate the rheology of a dilute suspension of aggregates with complex shape suspended in a non-Newtonian fluid by direct numerical simulations. Aggregates made of primary spherical particles are built through a fractal-like model. The fluid is modelled by the power-law constitutive equation. The dynamics of a single particle in an unbounded shear flow field is first computed. To this aim, finite element simulations are employed to calculate the angular velocity of the particle for several orientations on the unity sphere. The orientational dynamics is then reconstructed by integrating the kinematic equations for the orientation vector interpolating the angular velocity field. The first-order contribution to the viscosity is finally computed by means of a homogenization procedure. The effect of particle morphology and power-law index on the suspension viscosity is investigated.

Wednesday 11:40 Virtual / Track 7 CF2

Transport dynamics of microparticles in inertio-elastic vortex flows

Noa Burshtein[1], Arash A. Banaei[2], Simon J. Haward[3], Amy Q. Shen[3], Luca Brandt[2], and Anke Lindner[1]
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The dynamics and transport of microparticles (MP) are important in biological flows and for numerous applications in industry. In recent years, due to plastic degradation, MP is also becoming a significant health risk as their abundance rises in the marine environment. A large portion of MP is concentrated in the sea surface microlayer (the upper 1 mm of the ocean) where they are suspended in dissolved organic matter which contains polymers and surfactants with distinct non-Newtonian properties. Although oceanic flows tend to be turbulent and are expected to be homogenously mixed, there are various indications from field observations, experiments and numerical simulations which demonstrate that, depending on fluid and particle properties, MPs preferentially concentrate in specific areas of the flow field. To understand the underlying mechanisms affecting MP distribution in weakly elastic turbulent flows, we disentangle their response to a single element of the flow field, a single vortex. For this purpose, we use a microfluidic cross-slot geometry, to generate a stationary three-dimensional streamwise vortex at moderate Reynolds numbers. The well-controlled vortical flow field allows studying the transport and dynamics of neutrally buoyant MP suspended in Newtonian and weakly elastic fluids. The experimental results are complemented with numerical simulations and show that MP distribution in a vortical flow field can be highly influenced by the addition of small quantities of flexible polymers to the fluid. Although the fluid elasticity is weak, and the Stokes number is small (particles are expected to follow the streamlines of the flow) the elastic effects lead to distinctly non-homogeneous particle distributions in the vortical flow fields, resulting in absence of particles within the vortex core. This study provides a fundamental contribution to the study of MP-flow interactions and for the improvement of particle sorting and transport techniques with possible environmental and industrial applications.

Symposium FI

Flow instabilities

Organizers: Sandra Lerouge and Mahdi Davoodi

Wednesday 9:20 Virtual / Track 8 FI6

Asymmetric flows of complex fluids past a cylinder in a microchannel

Stylianos Varchanis[1], Cameron C. Hopkins[1], Amy Q. Shen[1], John Tsamopoulos[2], and Simon J. Haward[1]

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We investigate the formation of steady, laterally asymmetric flow patterns during the flow of various complex fluids past a rigid cylinder confined in a microchannel. Initially, we employ three model polymeric solutions to investigate the effect of their rheological properties on the onset of flow asymmetry: 1) A strongly shear-thinning but inelastic Xanthan gum solution, which is modelled with the Carreau-Yasuda generalized Newtonian model, 2) a strongly elastic but non-shear thinning PEO solution, which is modelled with the FENE-CR model, and 3) a both elastic and shear-thinning PEO solution, which is modelled with the linear Phan-Thien and Tanner model. Using numerical simulations and microfluidic experiments, we find that laterally asymmetric flow configurations can be supported only when the fluid exhibits both elastic and shear-thinning effects; in the absence of either, the flow remains laterally symmetric. The proposed physical mechanism suggests that strong elastic stresses on highly curving streamlines at the wake of the cylinder, combined with shear-thinning effects on the wall of the channel, give rise to a supercritical pitchfork bifurcation and flow bi-stability. Increasing the flow rate leads to gradually stronger flow asymmetry, with more fluid preferring to pass around one side of the cylinder. However, at very high flow rates an interesting re-symmetrization of the flow emerges, driven by a subcritical pitchfork bifurcation. This phenomenon is attributed to the disappearance of shear-thinning effects, as the shear viscosity of the fluid on the wall of the channel approaches the high shear rate plateau. Finally, we extend our analysis to wormlike micellar solutions (WLM) to examine how breakage and reforming of the micelles, as well as shear banding, influence the development of lateral flow asymmetry. The choice of a proper constitutive equation for WLMs that can describe the experimental data is also discussed.

Wednesday 9:40 Virtual / Track 8 FI7

Tristability in viscoelastic flow past side-by-side microcylinders

Cameron C. Hopkins, Simon J. Haward, and Amy Q. Shen

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Viscoelastic flows through microscale porous arrays exhibit complex path-selection and switching phenomena. However, understanding this process is limited by a lack of studies linking between a single object and large arrays. Here, we report experiments on viscoelastic flow past side-by-side microcylinders with variable intercylinder gap. With increasing flow rate, a sequence of two imperfect symmetry-breaking bifurcations forces selection of either one or two of the three possible flow paths around the cylinders. Tuning the gap length through the value where the first bifurcation becomes perfect reveals regions of bi and tristability in a dimensionless flow rate-gap length phase' diagram.

Wednesday 10:00 Virtual / Track 8 FI8

Tomographic PIV measurements of viscoelastic instabilities in a glass 3D micro-contraction

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Viscoelastic flow through an abrupt planar contraction geometry above a certain Weissenberg number (*Wi*) is well known to become unstable upstream of the contraction plane via a central jet separating from the walls and realizing counter-rotating vortices in the salient corners. Here, for the first time we consider three-dimensional (3D) viscoelastic contraction flow in a microfabricated glass square-square abrupt contraction geometry. We employ state-of-the-art microtomographic PIV to produce time-resolved and volumetric quantification of the 3D viscoelastic instabilities arising in a refractive index-matched glycerol-water-polyacrylamide solution driven through the geometry over a wide range of *Wi* but under conditions of negligible inertia. Based on our new measurement and analytical techniques, we describe new insights into the growth, propagation, and transient dynamics of an elastic vortex formed upstream of the 3D micro-contraction. We observe a new growth plateau region of the corner vortices whereby for increasing *Wi*, the vortices grow statically, then steadily oscillate at increasing frequency at a constant amplitude, then increase in amplitude. In addition, we report new out-of-plane asymmetric vortex behavior with a phase-wise dependence on *Wi*.

Wednesday 11:00 Virtual / Track 8 FI9

Linear Mechanisms for Transition in Rectilinear Viscoelastic Shearing Flows

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We show that pressure-driven plane and pipe Poiseuille flows of an Oldroyd-B fluid are linearly unstable for sufficiently high elasticities, in contrast to the Newtonian scenario wherein pipe flow is linearly stable for all Reynolds number (Re). The unstable mode in both cases is a "center mode" with phase speed very close to the base state maximum, and is believed to underlie the dynamics of the recently identified elasto-inertial turbulent regime. The critical Reynolds number (Re_c) for the onset of the elasto-inertial center-mode instability is a function of the elasticity number E and solvent-to-solution viscosity ratio β. For both pipe and channel flows, for finite 1-β, Re_c decreases as $E^{-3/2}$ for small E, approaching a minimum, before diverging sharply beyond a critical E. For pipe flow, this trend continues in the limit β approaching 1, with E(1-β) replacing E, and the minimum Re_c approaching a value of O(60). However, for channel flow, Re_c continues to decrease with increasing E(1-β) for β approaching 1, with the original elasto-inertial instability morphing into a purely elastic instability, characterized by Re_c proportional to $(E(1-\beta))^{-1}$ in the limit E(1-β)>>1. An independent analysis shows that inertialess plane Poiseuille flow is indeed unstable for $\beta > 0.9906$ and W proportional to O(1000), with W(1-β) being the threshold parameter for β approaching 1. This is therefore the first discovery of a linear elastic instability in a rectilinear shear flow in the absence of inertia. The underlying elastic-critical-layer-mediated mechanism signals a marked departure from the prevailing notion that regards streamline curvature, and the associated hoop stresses, as an essential ingredient for purely elastic instabilities.

Wednesday 11:20 Virtual / Track 8 FI10

Edge fracture instability of viscoelastic liquid bridges

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Short liquid bridges are stable under the action of surface tension. In applications like electronic packaging, food engineering and additive manufacturing, this poses challenges to the clean and fast dispensing of viscoelastic fluids. Here, we investigate how short viscoelastic liquid bridges can be destabilized by torsion. We consider a setup consisting of a liquid bridge confined between two concentric circular plates, one of which is rotatable. By combining high-speed imaging and numerical simulation, we show that the concave surface of a liquid bridge can localize shear, which in turns localizes normal stress and makes the surface more concave. Such positive feedback creates an indent which propagates towards the center and leads to breakup of the liquid bridge. For capillary stable bridges, such indent propagation causes the neck radius of the liquid bridge to undergo power-law decay. During the power-law decay, the relationship between the second-normal stress difference and the Laplace pressure at the indent tip meet the Tanner-Keentok criterion. This provides evidence that the indent propagation is caused by edge fracture, an often undesired viscoelastic flow instability characterized by the sudden indentation of the fluid's free surface when the fluid is subjected to shear. By edge fracture, even short, capillary stable liquid bridges can be broken in the order of 1 s. This may lead to new dispensing protocols that reduce substrate contamination by the satellite droplets and long capillary tails formed by capillary retraction, the current mainstream industrial method for destabilizing viscoelastic liquid bridges.

Wednesday 11:40 Virtual / Track 8 FI11

Side branched patterns, coalescence and stable interfaces during radial displacement of a viscoelastic fluid

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The dynamics of the interface when a Newtonian fluid displaces a dense viscoelastic fluid in a radial Hele-Shaw cell is studied. Increasing the ratio of viscosities of the two fluids and the elasticity of the outer viscoelastic fluid lead to a remarkable suppression of interfacial instabilities. While the morphologies and development of large-scale patterns are determined by elasticity and viscosity ratio, the onset of the interfacial instability can be correctly described by performing a linear stability analysis of the interface, considering viscosity ratio as the only control parameter.

Symposium MP

Multiphase and other complex fluids

Organizers: Mario Minale and Dganit Danino

Wednesday 9:20 Virtual / Track 9 MP6

Influence of egg yolk addition on rheological properties of linseed oil-based paints

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Egg yolk has been used in artistic paintings as binder since Antiquity and remained the primary medium for South-European panel painting in the Middle Ages, in the artistic technique named "tempera". Hypotheses have been made that later it was also used in order to change the rheological properties of the paint from tempera to oil paints, although very little experimental evidence is available on this. Fundamental work has to be done to correlate rheological parameters and properties relevant for painting with the final appearance of the paints we can observe in museums. This study will focus on the understanding of the role of egg yolk addition on flow properties of oil paints. Three types of paints based on oil and pigments (lead white or ultramarine blue) have been prepared: paints made from pigment and oil, paints made from pigment particles which are coated with dried egg yolk and dispersed in oil, and "tempera grassa" paints made from fresh egg yolk (incl. ca 30% water after paint preparation), oil and pigments all dispersed together. We will discuss and compare the effect of egg yolk on the flow properties of these different kind of wet paints. We will focus on the yield stress and complex shear modulus, which are influencing the "impasto" of a paint. In addition, the distribution of egg yolk and oil in "tempera grassa" paints was determined using fluorescence microscopy to gain insight into the structure of the paints. The effect of egg yolk coating on particle agglomeration was also investigated for better understanding of the flow behaviour of such artist paints. Finally, we will also discuss how the way of introducing the egg yolk affects drying and curing of the different kinds of paint.

Wednesday 9:40 Virtual / Track 9 MP7

Influence of lead driers on artistic oil paint rheological properties

Lucie Laporte[1], Arnaud Lesaine[1], Guylaine Ducouret[2], Frédéric Gobeaux[3], and Laurence de Viguerie[1]
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Artistic painters have prepared paint mixtures, since the 15th century, by adding oil binder to various pigments. Oils commonly used in historical paintings are called drying oils: they exhibit natural hardening properties after a long period of exposure to air. To accelerate the oil drying process, numerous historical recipes mention the use of inorganic drying compounds (or "driers"), *e.g.* lead oxide (PbO). The driers are ground, added to the oil and the mixture is heated, possibly with water. This treatment induces changes of the paint properties.

The present work thus aims to characterize the modifications induced by the formulation of the paint mixture at the molecular and supramolecular level. More specifically, the flow properties of treated oils at a macromolecular level will be correlated to their organization on a supramolecular scale.

We have formulated oils based on recipes from the 17th to the 19th century: our systems consist of linseed oil, widely used by painters, and lead oxide. The saponification of triglycerides during heating was monitored by infrared spectroscopy: the formation of lead soaps modifies the physicochemical properties of oils, whose rheological behavior has been characterized. Linseed oils cooked with 0-10% PbO behave like Newtonian fluids. With 20% PbO, metal soaps induce strong modifications of the rheological properties, leading to viscoelastic systems with shear thinning behavior. This suggests a structuration of the system at the supramolecular scale, that can be disrupted by shearing and which partially restructures within a few hours. In parallel, SAXS (Small Angle X-ray Scattering) measurements revealed the presence of lamellar phases with a characteristic distance of the order of 5nm in the viscoelastic samples. Finally, rheo-SAXS measurements will be carried out to elucidate the supramolecular organization of treated oils under shear and to link it to the different stages of paint application.

Wednesday 10:00 Virtual / Track 9 MP8

Thermo-rheological behaviour of modified asphalt binders with recycled plastomers and plastomers-graphene mixture compared with SBS Polymer-Modified Bitumen

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Bituminous pavements constitute a major part of the paved area in most parts of the world. The initial cost is very low, but bituminous pavements are subjected to distresses during service life. The typical phenomena are rutting, fatigue and low-temperature cracking. In recent times, due to increased overloading in vehicles and global warming, the distresses are much more present. These problems cause also an increment in the maintenance cost of the roads. Then, because it is notorious that the typical pavement distresses are related to the rheological bitumen properties, a series of modifications have been made during the last years and elastomers, polymers and nanomaterials are added to improve the viscoelastic behaviour, the strength, and the rate of plastic deformation. The well-accepted modifier is the styrene-butadiene-styrene (SBS) wich after incorporation, creates a biphasic system and at the moment results to be one of the best modifiers. Nowadays, researchers are trying to substitute SBS and/or virgin polymers with recycled polymers and nanomaterials. Even if the mechanical properties of recycled plastic is poorer respect to the new polymer, this type of approach is also supported by recycled plastics because reuse the waste is eco-friendly. In the last few years, one of the most popular nanomaterial added to bitumen is the Graphene, because recently it is possible to obtain it at lower cost respect to the past and a lot of studies have demonstrated its potentiality as a modifier. On the light of the above, rheological characterization of virgin bitumen with and without SBS was compared with bitumens modified with recycled plastomers and with a mixture of plastomers and graphene. The evolution of the thermal and rheological behaviour of the different samples has been followed by steady and oscillatory shear tests and dynamic mechanical thermal analysis (DMTA).

Wednesday 11:00 Virtual / Track 9 MP9

Evidence of Strain-Induced Violation of Thermodynamic laws in mesoscale Liquids

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Thermo-elasticity couples the deformation of an elastic (solid) body to its temperature and vice-versa. It is a solid-like property. Highlighting such property in liquids is a paradigm shift: it requires long-range collective interactions that are not considered in current liquid or viscoelastic descriptions. We present pioneering studies providing evidence for such solid-like correlations. We will show that ordinary liquids (glycerol, Polypropylene glycol...) emit modulated thermal hot and cold signals when applying a low frequency (Hz) mechanical shear stress [1]. The thermal wave reaches a sizable amplitude. Thus, the liquid is able to convert the energy of shear waves in non-uniform thermodynamic states. These dynamic thermal changes support the hypothesis of the excitation of macroscopic shear elasticity which range is limited to small scale, in accordance with recent non-extensive theoretical models [2,3] and the identification of the generic sub-millimeter shear elasticity revealed in polymer melts, glass formers, ionic liquids and molecular liquids a couple of years ago [4].

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Wednesday 11:20 Virtual / Track 9 MP10

Rheological properties of the rotator phases of alkanes

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The simplest organic molecules, alkanes, with intermediate chain lengths *ca.* 10-50 C-atoms, are known to crystallize by passing through intermediate phases called rotator phases.[1] Five different in structure rotator phases are known to form depending on the alkane chain length. Molecules arranged in rotator phase possess a long-range positional order while preserving certain mobility to rotate around their long axis. This results in a complex visco-plastic rheological behavior which plays a key role for processes observed in living and non-living nature, for example in disperse systems[2], lubricants and for the mechanisms of cuticle self-healing in plants.

The phase transitions between the different rotator phases are traditionally studied using X-ray scattering (SAXS/WAXS) or calorimetric measurements (DSC). In the current study we developed a procedure allowing us to distinguish the phase transitions between the separate rotator phase using rheological measurements. Furthermore, the visco-plastic properties of the rotator phases were determined and compared with respect to the alkane chain length. We show that the main contribution to the measured storage and loss moduli comes not from the arrangement of the molecules in the different rotator phases, but from the supercooling upon which a particular rotator phase is observed, *i.e.* the difference between the melting temperature of the respective alkane and the temperature at which the moduli are measured. The rheological behavior of several alkane mixtures was also studied and will be discussed in the talk with comparison to the behavior observed for the petroleum jelly, a hydrocarbon mixture widely used for lubrication and coatings.

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Wednesday 11:40 Virtual / Track 9 MP11

Enhancing magnetorheology under pulsed magnetic fields in saturation

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Magnetorheological (MR) fluids of interest in current applications are prepared by dispersion of magnetisable particles in (non-magnetic) liquid carriers. They exhibit a remarkable rheological change (so-called MR effect) upon the application of a magnetic field. The reason for this is the magnetic field-guided colloidal assembly of the dispersed magnetisable particles. The self-assembly can be controlled through the field configuration (DC, AC or combinations) and the strongest MR effect is achieved in saturating fields. A new device is constructed to measure the MR effect under homogeneous magnetic fields in saturation. The device optimization is done using magnetostatic Finite Element Method simulations. Also, Computational Fluid Dynamics simulations are performed and validated against experiments and theoretical calculations. Magnetostatic simulations on model dipolar lattices are carried out in a wide range of particle concentrations at saturation and results compared to experimental ones. Deviations between simulations and experiments are presumably due to a lower compactness and the presence of defects in the field-generated structures. This hypothesis is supported by particle level simulations and experiments under pulsed magnetic fields.

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Symposium PG

Powder rheology, granular flows and rheology of solids

Organizers: Alexandra Aulova and Stefan Gstöhl

Wednesday 9:20 Virtual / Track 10 PG6

Intermittent flow and transient congestions of soft spheres in silo discharge

Jing Wang[1], Kirsten Harth[1], Ralf Stannarius[1], and Tamás Börzsönyi[2]

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Soft, low-friction particles exhibit very peculiar features during their discharge from containers with narrow orifices. Their outflow rate and the clogging probability both depend upon the momentary silo fill height, in sharp contrast to silos filled with hard grains. One reason is the fill-height dependent bottom pressure. This pressure does not saturate by the Janssen effect at fill heights typically used in our experiments. We study the statistics of silo discharge of soft hydrogel spheres, with elastic moduli of the order of 50 - 100 kPa. Their outflow rate becomes increasingly fluctuating and even intermittent with decreasing orifice size. In orifices narrower than two particle diameters, outflow can stop completely for some transient periods, before the clogged state dissolves spontaneously after a couple of seconds and the discharge continues [1]. A similar behavior of non-permanent congestions has been described in literature for animals or pedestrians passing narrow gates or exits, but never for inanimate hard granular materials. This unusual behavior can be attributed to slow reorganization processes in the container caused by the viscoelastic character of the hydrogel grains. We also show that the addition of small amounts (few percent) of hard, inelastic grains can have dramatic consequences for the outflow characteristics, clogging probabilities and structures of the blocking arches at the orifice. Experiments are reported for a quasi-twodimensional container with a thickness slightly larger than the particle diameter. The outflow is recorded by means of high-speed video imaging, and at the same time, the mass of discharged material is recorded as a function of time using an electronic balance below the outlet.

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Wednesday 9:40 Virtual / Track 10 PG7

Fabrication of 2D dense suspensions of soft particles in microfluidic channels

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Soft Particle Glasses (SPGs) are ubiquitous, with industrial examples such as emulsions, gels, and pastes. To properly understand the macroscopic response of soft particle glasses to stress/strain, an understanding of the relationship between material microstructure and its dynamics upon exposure to stresses is required. However, it is notoriously difficult to study the effects of particle softness on this relationship because changes in particle Young's modulus inevitably leads to changes in other properties such as the friction coefficient, surface roughness, and/or interparticle adhesion. Here, we present an experimental system based on 2D hydrogel ensembles that circumvents this issue. The system is based on the in-situ fabrication of poly(ethyleneglycol) diacrylate (PEGDA) hydrogel particles by UV-crosslinking. Changing the PEGDA concentration before crosslinking allows us to tune the Young's modulus by approximately 3 orders of magnitude without changing other particle properties. We are able to apply a compressive stress to the ensemble by flowing uncured solution over and under the particles and study the response of the ensemble over time. From these time-lapses, it is possible to extract several microstructural quantities, such as inter-particle forces and excess entropy, as well as several dynamical quantities, such as D^2_{min} and visco-elastic timescales. This experimental model system has the potential to provide key insights into the relationship between structure and dynamics of SPGs.

Wednesday 10:00 Virtual / Track 10 PG8

Magnetic resonance imaging (MRI) for the investigation of shear zones in soft granular particle ensembles

Zohreh Farmani[1], Jing Wang[2], Joshua A. Dijksman[1], Cindy Lübeck[2], Oliver Speck[2], and Ralf Stannarius[2]

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In order to understand the typical heterogeneous flow behavior of granular materials, it is important to combine rheological test geometries with three-dimensional imaging. A standard setup for continuous shear experiments is the plate-plate geometry where the material is sandwiched between a fixed and a rotating plate. An alternative is that of the split-bottom container with a free granular bed surface. In contrast to simple liquids, shear of granular ensembles is typically concentrated in narrow zones in each of these arrangements. We investigate, for the first time, the shear behavior of ensembles of soft, low-frictional spherical grains under shear. The characterization of the detailed shape of the localized shear zone with non-invasive techniques in opaque materials requires the use of tomographic techniques. For these experiments, hydrogel spheres are swollen in salted water to a size of 6 mm diameter. They are mixed with few percent of similar spheres swollen in a dilute $CuSO_4$ solution. The MRI scanner detects both types of spheres, but the copper sulfate doped particles provide a stronger MRI signal while those swollen without this dopant yield only a much weaker signal. The reason is the enormous reduction of T_1 by the dopant, which is beneficial when fast acquisition times are chosen. The doped spheres that appear much brighter in the tomograms can thus serve as probes for particle tracking. Similarly, one can employ particle imaging velocimetry (PIV) when samples consisting exclusively of doped spheres are employed. We record tomograms after stepwise rotation of one of the plates and determine the flow local field in different shear geometries.

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Wednesday 11:00 Virtual / Track 10 PG9

Flow study for poly-dispersed dense granular suspension in Non-Newtonian media, mimicking concrete flow

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The study of internal flow dynamics and associated particle migration for poly-dispersed dense granular suspension, e.g., flowing concrete, still lacks quantification on a single particle level. This includes the flow driven particle migration, like the formation of a lubrication layer [1]. The observation of flowing dense granular systems is often restricted by the opacity of the sample. Non-optical techniques, like ultrasonic velocimetry, have been used instead [2].

We use a macroscopically highly transparent model system for concrete and cement paste [3] that is a dense granular suspension of particles suspended in non-Newtonian media (particle volume fractions of 42% to 48%). The model system mimic the rheology behavior of cement paste (yield stress and plastic viscosity) and is completely index matched, allowing tracking of tracer particles at any given plane inside the flow. The rheological characteristics of the model system is tunable through its composition of additives.

We analyze gravity-assisted continuous flow for the model system through a cylindrical pipe. Our setup allows tracking of polydisperse tracer particles using diffused back-light illumination. The flow is observed at different sections of the pipe and near its wall. We quantify the flow induced particle migration by extraction of the particle trajectories normal to the wall. The flow analysis revels a flow profile similar to a plug flow and a migration of larger towards the central region of the flow. Sliding and rolling motion of the particles is observable. The lubrication layer thickness is also evaluated in the study.

The study is been funded by DFG under the ambit of priority program SPP2005.

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Wednesday 11:20 Virtual / Track 10 PG10

Rheology of elongated frictional granular particles

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We investigated the rheology of a 3-dimensional granular system consisting of frictional elongated particles by discrete element model calculations. We simulated a homogeneous shear flow of frictional spherocylinders, and calculated a number of rheological quantities. In the framework of the $\mu(I)$ rheology, the effective friction was a non-monotonic function of the aspect ratio for interparticle friction coefficient $\mu_p \leq 0.4$, while it was an increasing function for larger μ_p. We revealed the microscopic origin of this peculiar non-monotonic behaviour. We showed the non-trivial dependence of the velocity fluctuations on the dissipation regime, and traced back the behaviour of the normal stress differences to particle-level quantities.

Wednesday 11:40 Virtual / Track 10 PG11

The rheological properties of suspensions as the base for powder injection molding

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Suspensions are among the most popular objects for studying due to their great diversity and their importance for various technological and everyday applications. There is a scientific interest in the fundamental relationships between the structure and properties of this matter. Among other things, highly concentrated suspensions are the basic materials for powder injection molding which plays a considerable role in the production of metal and ceramic parts of small size and complex geometry.

The objects of our research were model systems based on aluminum powder dispersed in LowMW poly(ethylene glycol) and real systems for powder injection molding, in which aluminum oxide was used as a dispersed phase and a mix of polyethylene (HDPE) and paraffin was used as a matrix. The rheological properties of objects were investigated using the rheometer RS-600 (ThermoHaake, Karlsruhe, Germany). The experimental data of model systems with different volume concentrations allowed us to observe a complete picture of the suspensions rheological properties, from the dilute dispersions, which are simple liquids to the highly concentrated suspensions, which are solid elastic-plastic medium. Concentration range from 55 to 65 vol.% is of particular interest due to their using in powder injection molding. Such compositions based on aluminum oxide were prepared. The dependence of the rheological properties on the powder content, its dispersion and temperature was investigated. Based on the experimental data, the optimal powder content and processing modes for the injection molding were selected. Of special interest is the use of these compositions for 3D printing. A filament with a stable diameter of 1.75 mm was produced and afterwards some parts was printed by means of a printer based on fused filament fabrication (FFF) technology.

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Symposium MN

Micro and nano fluidics and microrheology

Organizers: Anke Lindner and Laura Casanellas

Wednesday 9:20 Virtual / Track 11 MN6

Hydrodynamic and viscoelastic effects inside a biomimetic array of passive cilia-like structures

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How the beating of cellular cilia in a surrounding fluid gives rise to fluid transport and coordinated cilia motions is a 70-year-old problem, but it remains an open question due to the complexity and the diversity in the length scale of the phenomenon involved. Theoretical studies [1] suggest that the non-Newtonian hydrodynamic coupling between cilia plays a crucial role. This consideration asks for a systematic study of the non-Newtonian effects on large arrays of passive slender objects. Yet, no such experimental investigation has been conducted because of the technological difficulties. Here we combine two cutting edge microfabrication technologies, the Nanoscribe platform [2] that allows to fabricate large arrays of soft and flexible structures with micrometric scale (d = 2 um, h=50 um); and the Lightfab 3D printer [3] for making glass microfluidics channels that are suitable to resist viscoelastic flows. We then conduct the first systematic, quantitative study of the interaction of a large array of micrometric passive cilia-like structure with non-Newtonian biopolymer solution (hyaluronic acid in water). The soft cilia-like structures bend under flow. Under increasing flow rates (from 0 to 1 mL/min), we first observe successively the unsynchronised oscillation of the structures, followed by the emergence of a metachronal wave that propagates through the array, and finally the apparition of two synchronised symmetric metachronal waves. We further propose a quantitative analysis of these phenomena to fully characterise the instabilities at play and discuss how these metachronal waves relate to the ones observed in biological systems.

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Wednesday 9:40 Virtual / Track 11 MN7

Lingering dynamics of microvascular blood flow in vivo

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The microcirculation in animals and humans is directly linked to their health state. Any alterations in this blood flow may lead to pathological states, e.g. ischemia. Since typical vessel dimensions in the capillary bed are in the range of individual red blood cells, the particulate nature of blood is well pronounced. Indeed, red blood cells undergo a complex shape transition while flowing through bifurcating and merging vessels.

While approaching a bifurcation apex, red blood cells can drastically reduce their velocity, and even rest at this apex. These so-called lingering events are well-known in the field of hemodynamics, however, no systematic studies concerning the effects on the subsequent bloodstream exist.We present an experimental study on living hamsters investigating the lingering events and consequences thereof. Therefore, we perform a joint method of particle tracking and integrated signal evaluation of flowing red blood cells. We show evidence that lingering events lead to a shift of median durations of cell-free areas. Further, lingering events can be linked to the redistribution of consecutive red blood cells in the bifurcating geometry as well as a spatial distancing of red blood cells.

Wednesday 10:00 Virtual / Track 11 MN8

Optimisation of hyperbolic microchannels for the characterisation of bio-particles mechanics

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Bio-particles transported in viscous flows have a large range of dynamic behaviour, including morphological transitions, orientation dynamics or deformations. The characterization of such complex dynamics under well controlled flows is essential to understand the mechanics of microscopic biological particles but also the rheology of their suspensions. While generating regions of simple shear flow in microfluidic devices is relatively straightforward, generating straining flows in which the strain rate is maintained constant long enough to observe the evolution of objects' morphology remains a technical hurdle. Here, we coupled an innovative approach based on optimised design of microfluidic converging-diverging channels coupled with a microscope-based tracking method to characterise the dynamic behaviour of individual bio-particles under homogeneous straining flow. The tracking algorithm, combining a motorised stage and a microscopy imaging system controlled by external signals, allows the transport of individual bio-particles over long-distances with accurate resolution on the image to be monitored. This experimental implementation of the numerically optimised microchannels clearly shows the ability of this approach to provide linear velocity streamwise gradients along the centreline of the device, allowing for extended consecutive regions of homogeneous elongation and compression. We followed the transport of three different bioparticles (DNA, actin filaments and protein aggregates) in channels with this design to highlight the ability of our approach for investigating dynamics of objects with a wide range of sizes, characteristics and behaviours of relevance in the biological world.

Wednesday 11:00 Virtual / Track 11 MN9

Extraction of diffusion coefficient and anomalous exponent from the MSD, log-log versus (non)linear fitting

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Tracking of small particles undergoing a Brownian motion is a widespread method in passive microrheology. The averaged mean squared displacement (*MSD*) is extracted from particle positions. A generalized approach $MSD(\tau) = 2nD_\alpha \tau^\alpha$ is frequently used to extract the diffusion coefficient D and the anomalous diffusion exponent α by fitting experimental or numerical data where least squares are minimized. A common suggestion is to perform the fitting from the logarithm of the data, a linear regression in log-log plots respectively [1].

We demonstrate that those procedure leads to a small but systematic underestimation of the extracted parameters with respect to the nonlinear regression of the non-transformed data. Our results are supported by simulations of simple Brownian motions. In addition, we show analytically this parameter under/overestimation for almost any data transformation and subsequent least square fitting.

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Wednesday 11:20 Virtual / Track 11 MN10

Thermo-mechanical coupling in mesoscopic liquids

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Thermoelastic effects have been so far established and understood for solids only [1]. Under periodic strain loading, the temperature oscillates, implying that the medium is under stress. For liquids, a thermal study should be ineffective when probing the low frequency liquid dynamics [2]: the low frequency excitation (0.5 - 5 rad/s) is much slower than any known relaxation time ($1/f \ll t_{relax}$) [3]. In our work, we investigate the thermal response of ordinary liquids under mechanical shear strain in mesoscopic scale (100 - 250 μm). Particularly, we study glycerol and polypropylene glycol (PPG) at room temperature far away of any critical temperature. Two series of mechanical measurements were carried out: low frequency oscillatory shear strain and step shear strain. We observe in both cases a significant thermal response. Upon oscillatory mechanical shear, the liquids emit a modulated hot and cold signal synchronous with the applied excitation [4]. For step strain measurements, we observe a fast thermal response upon strain loading followed by a long (several seconds) thermal relaxation. Our observations highlight a thermomechanical effect in liquids, which is only possible by assuming elastic-type interactions at microscopic length scales. These new findings agree with new theoretical models that interpret the macroscopic liquid behaviour as an asymptotic branch where, at a smaller scale, liquid molecules behave elastically with suppressed relaxations and where the dynamic role of intermolecular interactions is central [5,6].

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Symposium CS

Colloids and suspensions

Organizers: George Petekides and Valeria Garbin

Wednesday 9:20 Virtual / Track 12 CS34

The effects of shearing and extensional flows on the alignment of colloidal rods

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Cellulose nanocrystals (CNC) can be considered as model colloidal rods and have practical applications in the formation of soft materials with tailored anisotropy. Here two contrasting microfluidic devices are employed to quantitatively elucidate the role of shearing and planar extensional flows on the alignment of a dilute CNC dispersion. Characterization of the flow field by micro-particle image velocimetry is coupled to flow-induced birefringence analysis to quantify the deformation rate-alignment relationship. The deformation rate required for CNC alignment is 4 times smaller in extension than in shear. The birefringence signal rising from the CNC alignment in shear and extension can be scaled on a single master curve using a Péclet number that accounts for the shear and extensional viscosity of the solvent fluid, respectively. Based on this simple scaling concept it is thus possible to anticipate the alignment of rigid colloidal rods under extensional deformation by knowing the respective alignment profile in a shearing flow accessible via multiple rheo-optical techniques. Quantification of the differences between shearing and extensional kinematics at aligning colloidal rods establishes coherent guidelines for the manufacture of structured soft materials.

Wednesday 9:40 Virtual / Track 12 CS35

Distinguishing Thixotropy from Viscoelasticity

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Recently there has been a debate in the literature on what constitutes thixotropy and how to distinguish the same from viscoelasticity. In this work, we assess various protocols proposed in the literature to distinguish thixotropy from viscoelasticity. To facilitate such distinction, we use a model viscoelastic material (aqueous solution of Polyethylene oxide) and a viscoelastic constitutive equation (FENE-P model) as well as a model thixotropic material (aqueous dispersion of clay) and a structural kinetic model based on free energy that shows thixotropy. We observe that with an increase in relaxation time of a viscoelastic material, it becomes exceedingly difficult to differentiate between a viscoelastic and thixotropic response.

Wednesday 10:00 Virtual / Track 12 CS36

Full rheological characterization of commercial graphene-based inks

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Printed electronics refers to the application of printing techniques to a functional ink to fabricate electronic structures, devices and circuits. The portfolio of printing techniques comprises a wide range of methods. Finding the right balance between printability and functionality has always been one of the biggest challenges for printed electronics[1]. The rise of graphene may foreshadow the next generation of printed electronics. New graphene-inks are yearly coming to the market place, however, their printability still needs to be fully understood in order to scale-up towards to Industrialization[2].

Inkjet printing is considered the most promising technique for printed electronics. Inkjet processing is very sensitive to the formulation of the inkjet fluid and, particularly, to the presence of solid particles. In order to understand the dynamics of the inkjet processes (drop-on-demand or continuous inkjet), one requires a deep understanding of the capillary breakup phenomena and of the rheology of the inkjet fluids. Capillary break-up extensional experiments have proved effective in measuring the elongational properties of polymeric fluids and particulate suspensions; however, there is relatively little known about particulate effects on the stability and break-up of liquid jets[3], and even less for 2D-particle-laden fluids[4].

In this study a full rheological characterization of three different commercial graphene-based inks has been performed under simple shear and uniaxial extensional flow in the Capillary Breakup Extensional Rheometer. Additionally, the influence of an external electric field on the rheological behaviour of the inks has been also explored[5].

Acknowledgement: This work was financially supported by FCT through project PTDC/EME-APL/30765/2017 - POCI-01-0145-FEDER-030765.

Refs: [1] Nature Nanotechnology 12, 283 (2017). [2] Nat Nanotechnol 12, 343-350 (2017). [3] PoF 26, 033101 (2014). [4] JoR, 64(1), 81-93 (2020). [5] JoR, 64(1), 43-54 (2020).

Wednesday 11:00 Virtual / Track 12 CS37

Shear-induced glass-to-crystal transition in anisotropic clay-like suspensions

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We report and elucidate a rarely observed glass-to-crystal transition happening upon flow cessation, after a period of shear, in a system of anisotropic clay-like colloids. We first present a new simulation strategy to study the structure evolution and mechanical response of anisotropically charged, plate-like colloids to a shear flow. Hydrodynamics are computed using an extension of Accelerated Stokesian Dynamics for anisotropic objects, and electrostatics are accounted for with a site model including charge renormalization. We then briefly present the structures obtained in quiescent conditions as a function of volume fraction and salt concentration, and we confirm previous results obtained on clay-like systems with different numerical methods, in particular the existence of bonded or non-bonded glasses and different gel states. The main results of this work concern the study of partial orientational and positional ordering of initially glassy suspensions by shear and the subsequent evolution towards a nematic crystal upon flow cessation. The detailed mechanisms at play are elucidated by examining time-resolved statistical information on the structure and on the hydrodynamic and electrostatic stresses that develop as shear is started and stopped. The key for shear-induced partial ordering is the forced alignment of platelets upon shear startup, which unlocks translational degrees of freedom in the initially arrested state. Hexagonally packed strings of platelets are thus formed under shear. A crystal cannot be obtained at this point due to the continuous hydrodynamic forcing, but the flowing structure is then energetically sufficiently close to the crystal state for the latter to be reached after flow cessation. This mechanism involving a flow-induced weakening of the translation-orientation coupling could be actually quite generic for other suspensions of strongly anisotropic colloids interacting at long range.

Wednesday 11:20 Virtual / Track 12 CS38

The role of the water soluble organic carbon of soils on the stability of natural slurries

Raffaella Martone, Claudia Carotenuto, and Mario Minale
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Mudflows are real natural hazards; many studies have been performed to prevent these disasters. Triggering and evolution of mudflows depend on several factors, and one of them is the soil organic carbon (SOC) content. In previous studies, we analysed the stabilizing effect of the SOC on the rheology of natural soil-water slurries [e.g., Carotenuto et al., Earth Planet. Sci. 16:89(2016)]. We tested samples with their original SOC and with fractions of it, selectively removed with specific treatments. Mild treatments remove the dissolved organic carbon (DOC) which is the SOC water soluble fraction weakly linked to the soil mineral matrix, while strong treatments can act on the intimately linked SOC. Samples with similar granulometry and mineralogy were collected from two sites: one involved (Cervinara, South Italy-SOC=8,51g/Kg) and one never involved (Camposauro, South Italy-SOC=76,4g/kg) in a landslide. The yield stress and the viscosity of slurries can affect the mudflow trigger and propagation, respectively; we demonstrated that they both decrease by reducing SOC. DOC can stabilize the slurry made with Cervinara soil while it is less effective with Camposauro's one.

A rain can solubilize the soil DOC fraction. We here investigated the stability of a slurry prepared with soils subjected to different water-treatments: a) "wetted", b) "washed". In both cases the soil is immersed in water. In the case a), it is dried without spilling any liquid; in the case b), after the solid decantation, the clear liquid is spilled and then the sample is dried. We showed with rheological measurements and granulometric tests that it is enough to wet the soil to destabilize the slurry similarly to the case when the DOC is removed for Cervinara sample, while for Camposauro soil both water-treatments, though destabilizing the sample, do not act as the total DOC removal does. These results suggest that a soil prone to be involved in a mudflow can be destabilized by a meteoric event preceding the one that triggers the landslide.

Wednesday 11:40 Virtual / Track 12 CS39

Proving attraction nature on cementitious materials through oscillatory rheology

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Oscillatory rheology has proved a promising method to measure the nature of interactions between particles of inorganic materials [1]. One of the most widespread materials is Ordinary Portland Cement (OPC), for which interactions are known to be "strong-short-range attraction" [2]. Due to its substantial environmental impact, alternative materials such as Alkali-Activated Binders (AABs) have been developed since the 1930s [3], but are not well characterized yet.

In this work, oscillatory rheology is applied to both cementitious materials: OPC and AAB pastes are characterized and compared to a model material, a calcite suspension. The interstitial solution composition of the AAB is also varied (i.e. Ca^{2+} concentration). The elastic properties (elastic modulus and critical strain amplitude at which the paste yields) are measured as a function of volume concentration of particles, in a range for which an "attractive gel-like behavior" is observed [4]. The amplitude of this concentration range depends on the extension length of the interparticle forces, and on their nature. At first, we characterized the elastic domains (dominated by interaction forces) using a classic fractal model. Then, we extracted the fractal dimensions of the flocs formed upon self-assembly of the primary particles, using the method by Shi et al. [4].

We found that the nature of interactions in AAB is intermediate between cement and calcite pastes [5], explaining the difference in their fresh behaviors. Results suggest that the interstitial solution composition in AABs plays a key role in determining and optimizing their properties (i.e. surface potential, superplasticizer effect, setting time...).

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Wednesday Afternoon

Symposium CS

Colloids and suspensions

Organizers: George Petekides and Valeria Garbin

Wednesday 13:00 Virtual / Track 1 CS12

Rheology of Graphene Derivatives Suspensions on Yield Stress Fluid

Lorena C. Moraes[1], Mônica F. Naccache[1], Ricardo J. E. Andrade[2], and Helio Ribeiro[2]
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This work investigates the impact of graphene derivatives suspensions on the rheology of a yield stress fluid. The graphene derivatives used were graphene oxide (GO) and amino-functionalized graphene oxide (AFGO), nanomaterials made up of a graphene nanosheet having functional groups pending from their surfaces, the GO being composed of oxygenated groups and AFGO by amino groups. Such graphene derivatives have exceptional and very interesting physico-chemical properties, and have good dispersibility in water, organic solvents and polymeric matrices, providing great potential for the application of these nanosheets in composites and colloids. In this work we use an aqueous dispersion of Carbopol as the base fluid. It is a viscoplastic, transparent, non-toxic fluid, easy to handle, widely used in the pharmaceutical, and cosmetics industries. The effects of the concentration of both nanosheets, as well as the oxidation level of GO and amination of AFGO in the rheology of suspensions were investigated. Experiments were conducted in oscillatory and steady-state regimes. Both graphene derivatives have caused the perturbation of the hydrogel network, leading to the development of a weaker gel. All suspensions continue to behave as a yield stress fluid, but the increase in GO concentration leads to a decrease in the suspension viscosity, yield stress, and elasticity. Moreover, this decrease is much stronger when the GO presents lower oxidation levels. A time dependent behavior was observed only for the dispersion prepared with the higher concentration of GO 96h. For the AFGO suspensions, the higher is AFGO concentration, smaller are yield stress, viscosity, and elasticity. Also, AFGO with higher degree of amination causes a more pronounced drop in rheological parameters. In general, the oxidation and amination levels have a significant impact on the final rheological properties of this yield stress fluid. An investigation is currently being carried out on the rheological stability of suspensions during aging.

Wednesday 13:20 Virtual / Track 1 CS13

Rheological behavior of supensions of magnetic particles in polymer solutions

William R Suarez-Fernandez, Juan DG Duran, and Modesto T. Lopez-Lopez
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Even in the absence of crosslinking, long polymer strands have a strong influence on the rheological properties of composite media. In this work we investigate the effect that dissolved polymers have on the rheological properties of suspensions of iron particles in aqueous media. First, we investigate the role of sodium alginate (anionic polymer) of two different molecular weights: medium (120,000-190,000 g/mol) and large (up to 600,000 g/mol) molecular weight. Solutions of alginate with medium molecular weight demonstrated a liquid-like behavior (storage modulus -G'- less than the loss modulus -G") even at concentrations as high as 20% w / v, while the high molecular weight alginate solutions showed gel-like behavior (G' > G") at a concentration as low as 7% w / v. If medium molecular weight alginate was combined with chitosan (cationic polymer), a gel-like behavior (G' > G") was demonstrated, due to electrostatic attraction between oppositely charged polymers in aqueous media. Iron particles dispersed in these polymer solutions were trapped by entangled polymer strands, increasing stability against particle settling. Rheological analysis showed strong shear thinning behavior for these suspensions. More interestingly, the application of a magnetic field overcame the trapping of particles by polymers, leading to their migration and aggregation into structures aligned with the applied magnetic field, resulting in strong changes in the rheological properties. We analyze the role of the type of polymer in the rheological changes induced by the magnetic field under both stationary and oscillatory shear. Finally, we show that the use of the dimensionless Péclet number and inherent rheological parameters, highlights the differences between the samples and the experimental conditions. In all cases, as expected, at a sufficiently large shear rate, hydrodynamic forces governed the flow behavior of these suspensions of magnetic particles in polymer solutions.

Wednesday 13:40 Virtual / Track 1 CS14

Suspension of super-paramagnetic chains: dynamics and rheology under the combined effect of shear flow and rotating magnetic field

Emanuele Rossi[1], Jose A. Ruiz-Lopez[1], Adolfo Vazuez-Quesada[2], and Marco Ellero[1]
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The analysis presented in this study is related to the dynamics and rheology of a single as well as multiple chains composed by spherical super-paramagnetic beads [1]. The chains, suspended in a Newtonian fluid, showed a dynamic due to the combined effect of an external rotating magnetic field and a shear flow. According to two main non-dimensional numbers, the first, the ratio between the shear rate and the magnetic rotation frequency and, the second, the ratio between the hydrodynamic and the magnetostatic interactions, is possible to determine the viscosity throughout the analysis.

That means that, for shear rate smaller than the magnetic frequency the fluid surrounding the chain during its rotations appears accelerated, while the value of the viscosity suspension is lower than the solvent one. In the aforementioned regime shear-thickening can be observed. Moreover, for shear rates comparable to the rotation magnetic frequency, the viscosity value reached its maximum and non-linear coupling effects can be seen.
On the other side, for shear-rate values bigger than the rotation frequency, not only the viscosity decreased but a mild shear-thinning can be appreciated.

Obtained results shown that, related to the Mason number, the decreasing viscosity trend is in line with results available in literature regarding studies with fixed magnetic fields, in which the parameters resulting from the ratio shear-rate/magnetic-frequency produce a shift towards larger viscosity values. Similar as well as amplified observations arose also for higher concentrations using multiple chains [2].

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[2] Rossi, E., et al. Dynamics and rheology of a suspension of super-paramagnetic chains under the combined effect of shear flow and rotating magnetic field. Soft Matter. Under review.

Wednesday 14:40 Virtual / Track 1 CS15

Velocity-aligned stripes in field-driven anisotropic attractive suspensions

Jose R. Morillas[1], Óscar Martínez-Cano[1], Martin Cvek[2], Javier Ramírez[3], and Juan de Vicente[1]
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Unstable suspensions typically aggregate into vorticity-aligned stripes under steady shearing flows [1] because of the hydrodynamic coupling between the aggregates and the boundaries [2]. In this communication we demonstrate that velocity-aligned stripes can also be formed in unstable suspensions when attractive interparticle forces are strongly anisotropic. In particular, the model suspension used in this work is a magnetorheological fluid where attractive interactions can be externally controlled by the field strength of a superimposed magnetic field in the velocity gradient direction.

By using high-speed videomicroscopy and image analyses techniques we demonstrate that stripes form in a well-defined shear rate window. Stripes appear when the stress reaches a plateau in start-up tests. The lower critical shear rate corresponds to a critical Mason number close to one (i.e. balanced magnetostatic and hydrodynamic forces). The upper critical shear rate seems to be dictated by inertia. Both the mean separation distance of the structures and the mean width of the layers are insensitive to the shear rate and the field strength. Interestingly, a linear dependence is found with the gap. This linear dependence is captured by energy minimization first principles using magnetostatics simulations in model structures of finite size.

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Wednesday 15:00 Virtual / Track 1 CS16

Magnetorheology of Janus Particle Suspensions

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Magnetorheological (MR) suspensions are a complex class of fluids which show tunable and reversible phase transition from flowing state to solid-like behaviour by applying an external magnetic field. In this study, we analyze, for the first time, the yield behaviour of a MR suspension comprised of magnetic Janus particles. We compare the rheological characteristics of these suspensions with the more conventional homogeneous magnetic particles. MR suspensions are prepared by adding Fe_3O_4 capped (Janus particles) or fully coated (homogenous) silica colloids to a Newtonian silicon oil as carrier fluid. Because the core of the particle is the same for both particles, our synthesis process enables exploring the effect of surface coverage and particle anisotropy on the rheological response of these MR suspensions. Under external magnetic field, particles are magnetized and form aggregates which develop larger values of yield stresses in both MR suspensions. However, different values of yield stresses are obtained in the case of the two suspensions. Unlike homogeneous magnetic particles, magnetic Janus particles form staggered and double-like chain structures due to non-homogeneity of magnetization. This is a consequence of the anisotropy introduced at the surface of these particles. We discuss our findings based on microrheological models considering size, magnetic saturation, and spatial distribution of magnetic particles. Our results demonstrate the impact that engineered surface properties of colloids have in controlling the macroscopic response of these MR suspensions. In addition to roughness and size, we demonstrate for the first time that surface coverage of the particle can be a useful tuning parameter for controlling MR suspensions rheology.

Symposium PM

Polymer melts and composites

Organizers: Maria Teresa Cidade and Juan de Vicente

Wednesday 13:00 Virtual / Track 2 PM12

Investigating the transition between polymer melts and solutions in non-linear elongational flow

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The Doi-Edwards tube model, coupled with relaxation mechanisms such as reptation, contour length fluctuation and constraint release, allows to quantitatively predict the linear viscoelastic properties of entangled polymers. However, for non-linear elongational flows, large discrepancies still exist today between theoretical predictions based on the tube model and experimental results. In particular, qualitative difference has been observed experimentally between the elongation viscosity of entangled polystyrene (PS) melts and solutions containing the same number of entanglements and exhibiting the same normalized linear viscoelastic behavior. The cause of this non-universality is often attributed to a monomeric friction reduction, or to an interchain pressure effect. The purpose of the present work is to conduct well-defined experiments to further investigate how the steady extensional viscosity of polymeric melts, solutions and blends varies with the concentration and with the molecular weight of the chains. To this end, we investigate the changes in extensional flow behavior going from polymer solutions to the melt state. The non-linear extensional responses of several long PS chains, both in the melt state and diluted in different polymeric matrices at different concentrations are measured with a filament stretching rheometer. These concentrations have been chosen to explore both entangled and unentangled states. This allows us to discuss the influence of concentration and molar mass on the steady state elongational viscosity to highlight scaling relationships.

Wednesday 13:20 Virtual / Track 2 PM13

High-temperature oscillatory rheometry: glass melt characterization beyond established viscometric fixpoints

Christopher Giehl[1] and Daniela Ehgartner[2]
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In the glass transition region, the visco-elastic properties of polymeric materials show characteristic thermo-mechanical behavior. Oscillatory rheometry is a means to characterize the rheometric glass transition temperature, which is affected by both the cooling rate and the applied frequency. Although having fundamentally different molecular structure, chemical compositions and glass transition temperatures, the rheological behavior of inorganic glass melts shows distinct similarities compared to polymeric materials. However, such high-temperature measurements are technically challenging.

This study presents first quantitative thermo-mechanical visco-elasticity measurements on a glass melt obtained from concentric cylinder high-temperature oscillatory shear rheometry. The measurements were performed on reference glass DGG 1 with a Furnace Rheometer System combined with an air-bearing DSR 502 measuring head (Anton Paar), and a $Pt_{90}Rh_{10}$ measuring geometry.

Isothermal measurements from 1200 to 650 °C confirm reference viscosity values and amplitude sweeps show that in this temperature interval the linearity limit of the linear visco-elastic range decreases from $\gamma=20$ to 0.02%. Frequency sweeps mimic Maxwell-type behavior and moduli increase continuously towards the rheometric glass transition (G" max, e.g. 778 °C at $\omega=10$ rad s^{-1}). Merging of isothermal frequency sweeps provides mastercurves by time-temperature superposition and enables calculation of relaxation times. This study confirms that glass melts mimic Maxwell-type behavior and high-temperature concentric cylinder rheometry is a suitable method for quantifying their visco-elastic properties. Moreover, this approach offers improved glass melt characterization beyond commonly used viscometric fixpoints, which disregard quantification of the dominant elastic fraction in the visco-elastic behavior of glasses below the rheometric glass transition temperature.

Wednesday 13:40 Virtual / Track 2 PM14

Start-up shear experiments as a tool to infer the structure and dynamics of gluten gel in water

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We investigate the nonlinear viscoelasticity of model gluten gel in water. We used the start-up shear at various rates, from 0.1 s^{-1} to 10 s^{-1}, and with different total deformations: 100 SU, 500 SU, 1000 SU and 2000 SU. Thus, transient responses are obtained for the same shear rate window but with changing the mechanical history of samples. The ratio between the maximum and steady stress ($\sigma_{Max}/\sigma_{Steady}$) and strain at the maximum stress (γ_{Max}) are analyzed for the above experimental conditions. The transient regime reveals that the gluten gel behaves as a branched polymeric system, with noticeable wakening as a function of the mechanical history. A master curve for $\sigma_{Max}/\sigma_{Steady}$ as a function of the accumulated mechanical energy is built. Below E_c, a critical energy value, $\sigma_{Max}/\sigma_{Steady}$ is equal to one. Data in this regime corresponds to the transient regime of samples with total deformation of 100 SU and 500 SU. However, exceeding E_c, the ratio $\sigma_{Max}/\sigma_{Steady}$ sharply increases. This regime corresponds to the transient regime of samples with total deformation of 1000 SU and 2000 SU. By considering an effective mesh size, extracted from SAXS measurements, the critical energy E_c is comparable to the binding energy of about two disulfide bonds or tens of H-bonds. Furthermore, plotting $\sigma_{Max}/\sigma_{Steady}$ as a function of shear rate for the different total deformations reveals that this ratio increases with higher total deformation and the data has a shear rate power law dependence that become stronger with total strain, suggesting the system weakening. Concomitantly, we found that $\gamma_{Max}=10$ for the different experimental conditions, suggesting a strong stretching. Finally, the shear rate dependence of both quantities exhibits the presence of two regimes (transition at a shear rate about $2s^{-1}$) only with higher total strains (1000 SU and 2000 SU), suggesting that higher mechanical energy is responsible for the appearance of new local dynamics in relation with structural changes in the system.

Wednesday 14:40 Virtual / Track 2 PM15

Cole-Cole Relation For Long-Chain Branching From General Rigid Bead-Rod Theory

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Empirically, we find that parametric plots of the imaginary versus real parts of the complex viscosity may depend neither on temperature, nor on average molecular weight. Moreover, for fixed polydispersity, these Cole-Cole curves amplify both rightward and upward with long-chain branching content. In this paper, we find that general rigid bead-rod theory [O. Hassager, "Kinetic theory and rheology of bead-rod models for macromolecular solutions. II. Linear unsteady flow properties," J. Chem. Phys. 60(10), 4001-4008 (1974)] can explain these rightward and upward amplifications. We explore the effects of branching along a straight chain in small-amplitude oscillatory shear flow. Specifically, we explore the number of branches, branch length, branch position and branch distribution.

Symposium IR

Interfacial rheology, emulsions and foams

Organizers: Anniina Salonen and Nikolai Denkov

Wednesday 13:00 Virtual / Track 3 IR12

Benchmark solutions for flows with rheologically complex interfaces

Mick A. Carrozza, Martien A. Hulsen, and Patrick D. Anderson

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Due to a large ratio of interfacial surface area to bulk volume, the rheological properties of the interface largely influence the structure and overall properties of multicomponent fluids. When applying flow to e.g. an emulsion, the material structure is continuously developing due to migration, deformation, break up and coalescence of drops that interact with each other and the surrounding fluid. The mutual coupling between the bulk phases and the (compressible) interface, interfacial transport phenomena and interfacial rheology, make these flow problems difficult to analyse theoretically and experimentally as well as numerically. A combination of approaches would be extremely useful for reliably predicting and controlling material properties. In [1] we described a general framework that was used to accurately benchmark our 3D finite element implementation of two-phase incompressible Stokes flow with rheologically complex sharp interfaces. In this talk, we would like to show how this model validation using the method of manufacturing solutions works, which can be applied to other flow problems and numerical methods using (in principle) arbitrary interface constitutive models. The results of our convergence tests for drop deformation with viscous, elastic and Kelvin-Voigt interfaces in simple shear and uniaxial extensional flow show higher-order convergence in space and time. Furthermore, the deformation and orientation of a suspended drop with a viscous interface in shear flow for different Boussinesq numbers agree with results from the literature, obtained with other discretisation methods. New benchmark results were presented for drop dynamics in shear flow with Kelvin-Voigt interfaces. Compared to a viscous interface, the drop deformation becomes smaller and the drop becomes less oriented in the flow direction if interfacial elasticity is added.

[1] M.A. Carrozza, M.A. Hulsen, P.D. Anderson, J. Non-Newtonian Fluid Mech. 286 (2020) 104436.

Wednesday 13:20 Virtual / Track 3 IR13

Lubrication properties of model dairy beverages: effect of protein and oil droplets

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Tribology has gained interest in the food industry as a tool to study textural attributes. It has been acknowledged that the lubrication properties of foods, in addition to rheological properties, play a significant role in determining texture perception or "mouthfeel". For example, dispersed fat droplets act as a lubricant in the mouth, and contribute to a creamy and thick sensation in fat-containing foods and beverages. A clear relation between specific sensory attributes and lubrication behaviour has not been established, especially for foods or beverages containing multiple components. Nutrition beverages are an example of complex foods, as they contain high concentrations of proteins, fats and carbohydrates. Therefore, we investigated how each component contributed to the lubrication properties of beverages and in future studies, how this affects textural attributes. In the present study, we studied the lubrication properties of model liquid dairy systems, containing whey protein (native or aggregated), casein, and/or emulsified fat. We found that whey protein aggregates (~247 nm) led to higher friction, in the boundary and mixed lubrication regime, than casein micelles with a comparable size (~207 nm). The friction coefficients decreased as the concentration for those proteins increased. Additionally, mixing whey protein and casein micelles led to higher friction. The lubrication behaviour appeared to be influenced by the morphology and hydrophobicity of the protein particles. In the case of emulsions, lubrication was dominated by the type of emulsifiers. The emulsions stabilized with soy lecithin showed lower friction coefficients than emulsions stabilized by whey proteins. When these oil droplets (~440 nm) were added to protein dispersions, the friction coefficients decreased strongly. The mechanism determining the lubrication properties of various systems will be discussed.

Wednesday 13:40 Virtual / Track 3 IR14

Decoupling shear and dilatational interfacial rheology for investigating complex fluid interface

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Interfacial structure and rheological properties are important in biological (e.g. lung surfactants) as well as many synthetic systems (e.g. emulsions) and understanding the structure-property correlation can help guide the formulation of these systems with targeted interfacial properties. Mixed flow fields, typical of classical Langmuir trough experiments, convolute the interpretation of interfacial dilatational rheology for interfacial systems with both finite surface shear and dilatational moduli. Attempts have been made to resolve the anisotropic state of stress into their pure forms, either by multiple measurements in the Langmuir trough [1] or through the use of a radial trough [2]. In this presentation, we describe the design and implementation of a new "Quadrotrough" to better approximate pure dilation or shear interface kinematics. The rheological capabilities of this interfacial trough are demonstrated through proof-of-concept experiments on stearic acid, a simple model system. This new instrument allows us to systematically step through pure shear and pure dilatational flow to investigate the path dependence of interfacial isotherms more clearly. We demonstrate the critical importance of decoupling flow fields for complex interfaces with finite shear and dilatational elasticity for ease of data interpretation. Combining the new Quadrotrough with both Brewster angle microscopy and neutron reflectivity provides detailed structural measurements of the interface at the mesoscale and nanoscale that elucidates the source of this path dependence. The potential for coupling this trough with microstructural characterization via neutron reflectivity will be discussed and future investigations are reflected on for instrument development.

References [1] Petkov, Jordan T., et al. Langmuir 16.8 (2000): 3703-3711. [2] Pepicelli, Martina, et al. Soft matter 13.35 (2017): 5977-5990.

Wednesday 14:40 Virtual / Track 3 IR15

Rheology of macro- and nano-emulsions in the presence of micellar depletion attraction

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This presentation demonstrates the effect of interdroplet interaction on the rheological behavior of oil-in-water emulsions (o/w) within a range of macro- to nano-droplet sizes and various volume fractions from dilute to concentrated regimes. Emulsions consist of silicone oil dispersed in highly concentrated sodium dodecyl sulfate solution to induce micellar depletion attraction between dispersed phase droplets. We determine the total interdroplet interaction from electrostatic, van der Waals, and depletion attraction contributions. The maximum force between droplets, obtained from total interdroplet interaction, is used to calculate the theoretical yield stress of emulsions. For highly concentrated macro- and submicron emulsions, the yield stress, σ_y, is scaled with $a^{-1.3}$, where a is droplet size. The nanoemulsion gels have a scaling of $\sigma_y \sim a^{-2.1}$, whereas the glassy nanoemulsions and highly concentrated nanoemulsions have $\sigma_y \sim a^{-0.2}$ and $\sigma_y \sim a^{-0.33}$ scalings, respectively. By decreasing droplet size, the Laplace pressure increases, whereas the interdroplet attraction decreases. The former increases the elastic modulus and yield stress of emulsions, and the latter phenomenon decreases them. While the change in interfacial energy dominates the change in rheological behavior of concentrated macro- to submicron regime, the increase in interfacial energy and decrease in interdroplet attraction are both significant in the nanoemulsions.

Wednesday 15:00 Virtual / Track 3 IR16

Interfacial micro- and macro- rheology of fractionated asphaltene

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A long-term challenge in some heavy oil processes is to efficiently break water-in-oil emulsions that are stabilized by a rigid film of asphaltenes adsorbed at the water/oil interface. Asphaltenes are a solubility class and contain a large variety of chemical species only some of which form rigid interfacial films. It is well understood that the higher elasticity of asphaltene film is implying the higher stability of the emulsions. In this study, interfacial rheology and elemental composition are measured and linked for two asphaltene fractions: one enriched with surface active asphaltenes and one depleted. Asphaltenes were extracted from an Athabasca bitumen. One fraction was obtained from the separated oil phase and the other from the emulsion phase of an aged and settled asphaltene stabilized water/heptol (model oil) emulsion. The emulsion phase asphaltenes, labeled Active (A), included the asphaltenes adsorbed at the water/oil interface and asphaltenes from the entrained continuous phase. The asphaltenes in the separated oil phase did not adsorb at the interface and are labeled Partially Active (PA). The interfacial properties of each fraction were assessed based on interfacial tension (IFT), dilatational rheology and interfacial micro-rheology measurements. The IFT and dilatational rheology measurements were performed in a drop shape analyzer on a pendant drop of the model oil surrounded by reverse osmosis (RO) water. The micro-rheology measurements were performed by adding fluorescent PS particles to a flat interface between RO water and asphaltene in model oil generated in a home-made setup. Multiple particle tracking was performed to extract particles mean square displacements. Interfacial tension measurement showed that the A fraction reduced IFT significantly while the PA fraction had a negligible effect, confirming the higher surface activity of the A fraction. The dilatational elasticity of the A fraction was on average 6 mN/m higher than that of the PA fraction in the range of frequencies considered

Symposium MS

Modelling and simulations

Organizers: Natalie Germann and Daniel Read

Wednesday 13:00 Virtual / Track 4 MS12

Stretching of Associating Polymers in Steady-State Flow

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We present a tube model for the Brownian dynamics of associating polymers, such as naturally-occurring silk proteins or synthetic amphiphiles, in extensional flow. The model captures reptation and contour-length fluctuations in exact agreement with the Likhtman-McLeish model, and confirms the analytical predictions for the 'sticky diffusivity' by Leibler-Rubinstein-Colby theory. In the non-linear regime, our model also captures the finite extensibility of the chain, as well as the stretch-induced opening of associating `stickers'. Our model predicts the stretch transition to be at a `sticky Weissenberg number', as expected. In steady state, i.e., below this transition, our model shows a remarkably broad distribution of chain stretch: while non-sticky polymers usually show a narrow Gaussian distribution, the sticky counterpart shows broad power-law tails. We argue this enables a strategy to control flow-induced crystallisation by stretching a small fraction of chains, rather than all of them. Our modelling approach suggests that a full control and understanding of this process requires a precise insight into the mechanism of sticker dissociation. In particular, i. in the non-linear regime direct sticker dissociation is expected to be much faster than the bond-swapping mechanism that is focussed on in most molecular-dynamics studies, and hence ii. the sticker activation energy measured in the linear regime may not be the relevant one in the non-linear regime.

Wednesday 13:20 Virtual / Track 4 MS13

Non-Equilibrium Thermodynamics Modeling of Wormlike Micellar Solutions

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Wormlike Micellar Solutions (WMS) share many properties with polymeric systems, such as entropic stresses. However, in contrast to polymeric systems, they break / reform under the action of the flow giving rise, among other things, to shear bands in simple shear flow---see, for example, Helgeson, et al., J. Rheol., 53, 727-756 (2009). A simplified representation of the wormlike micellar structures as two populations of long and short (half as big) Hookean dumbbell chains was developed by Vazquez et al., J. Non.-Newtonian Fluid Mech., 144, 122 -139 (2007) (VCM model). This involved empirical modeling of the shear-induced rupture and reformation kinetics. This empiricism was avoided when the dumbbell model was cast within a non-equilibrium thermodynamic framework by Germann et al., J. Non-Newtonian Fluid Mech., 196, 51-57 (2013); 207, 21-31 (2014); 232, 43-54 (2016) introducing a direct correction of the reaction rates to the macromolecular conformations (GCB models). However, as the more recent work of Adams et al., J. Rheol., 62, 1419-1427 (2018), has shown based on molecular dynamics data, all those dumbbell-based models are microscopically thermodynamically inconsistent.

In this work, we show that the microscopic inconsistency can also be detected macroscopically as a violation of the Onsager reciprocal relations. We also show that the thermodynamic consistency is recovered if a more detailed representation of the wormlike structure is followed for the longer micelles, namely representing them as Hookean trumbbells (i.e. 3 bead/2 spring-chains), following a suggestion in the above-mentioned Adams et al. work. In addition, explicit use of fluxes within the mass transfer in the non-equilibrium thermodynamics framework allows for more consistent modeling of stress-induced migration effects. We show how all these new developments affect the theoretical predictions in simple shear flow and cylindrical Couette flow and how they compare against the predictions obtained with previous models.

Wednesday 14:40 Virtual / Track 4 MS15

A thermodynamically consistent model of polymer disentanglement under flow

Benjamin E. Dolata and Peter D. Olmsted
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We formulate a thermodynamically consistent constitutive equation modeling the stretch, orientation, and disentanglement of a polymer melt under flow. Most prior constitutive equations do not explicitly track the evolution of entanglements, leavening them unable to model physical phenomena such as the diffusion of entanglements across the interface during the welding of adjacent polymer filaments. We overcome this limitation by developing explicit coupled evolution equations for the tube conformation tensor and number of entanglements. The conformation kinetic equation is inspired by the Rolie-Poly equation, and accounts for reptation, retraction, and convective constraint release. The evolution equation for entanglements is obtained by casting the kinetic equation of Ianniruberto and Marruci in a thermodynamically consistent form. In our model, entanglements are lost via alignment of the tube with the flow and Rouse retraction of the chain within the tube and are gained via curvilinear diffusion. Different approximations for the alignment tensor are compared. Model predictions for the stress and entanglement evolution are in good agreement with measurements from molecular dynamics simulations.

Wednesday 15:00 Virtual / Track 4 MS16

Flow-induced fractionation effects on slip of polydisperse polymer melts

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The slip behavior of several high-density polyethylenes with a broad range of molecular weights (MWs) and distributions (MWDs) including bimodal is studied. A slip model combining reptation theory (Ebrahimi et al., J. Rheology, 59, 885-901, 2015), surface (entropic) driven fractionation by concentration gradients (Ebrahimi et al., Physics of Fluids, 28, 093101, 2016), and flow-induced migration is formulated to predict the slip velocity of the studied polymers as a function of MW and MWD. The model predicts the flow curve, the MWD at the wall in relation to that in the bulk, and the slip velocity over a wide range of shear stresses using a set of molecular parameters characteristics to high-density polyethylenes (HDPE) (studied in the present work) and other linear polymers. The predicted slip velocity is also physically sound since its predictions lie between the minimum and maximum limits set by the lowest and highest molecular weight chains present in the system, taking into account polydispersity and weight ratios. The entropy and stress-induced migration of short chains toward the die wall lead to an increase in slip velocity due to the local (surface) variation in MWD, especially at high shear stresses. While surface fractionation has a minor effect on the slip of narrow to moderate MWD polymers (particularly unimodal), its role is significant for broad bimodal MWD polymers. The inclusion of both effects (concentration and flow gradients) accurately captures the slip velocity of broad MWD polymers.

Symposium FB

Food and bio-rheology

Organizers: Jan Engmann and Clément de Loubens

Wednesday 13:00 Virtual / Track 5 FB12

Microfluidics elaboration and characterization of whey protein microgels

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Soft particles such as gelatinised starch granules, plant cells or dairy microgels play an important role in the textural and sensorial properties of food suspensions such as thickened sauces, purees or stirred yoghurt. As their textural properties depend on the individual structural properties of the particles such as size, shape, and rigidity, producing food-grade particles with controlled structure could help to elucidate the structure-properties relationship. Spherical whey protein microgels with adjustable size are produced through microfluidic emulsification and their mechanical properties are characterized. In general, microgels mechanical properties are assumed to be identical to the rheological properties determined on their macroscopic counterparts. In this study, we compare the mechanical properties directly measured on individual microgels using a microfluidic device with the rheological properties determined on macroscopic gels prepared in the same physico-chemical conditions. Microgels are formed in two steps: (1) microfluidic emulsification of a whey protein isolate aqueous solution in sunflower oil and (2) gelation by acidification of the protein solution droplets. Particles size can be controlled varying the experimental conditions during the emulsification process while gel mechanical properties depend on the gelation mechanism and protein concentration. Microgels mechanical properties are characterized with two different procedures: (1) osmotic stress experiments are done by observing the size variation of trapped microgels in a microfluidic chip

while flowing a polymer solution of known osmotic pressure, and (2) compression of particles trapped in a tapered glass microcapillary is observed under different hydrostatic pressures to determine the deformation at equilibrium. From image analysis, the bulk and shear moduli of individual microgels are determined and compared with macroscopic gels moduli.

Wednesday 13:20 Virtual / Track 5 FB13

Whey protein–based systems: a rheological and microscopic characterization for different industrial uses

Francesca R. Lupi, Giulia Franco, Noemi Baldino, and Domenico Gabriele
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The lack of proteins intake is a serious problem for elderly people or for persons suffering from dysphagia, whereas the daily consumption for sportsmen and athletes must be higher with respect to the common consumer. In this work, the addition of whey proteins to water was investigated to analyse two kinds of applications: from one hand the characteristics of suspensions of proteins in their native state, and, from the other hand, the promotion of gels formation obtained by proteins denaturation thanks to thermal processing. In the first system, proteins act as thickening agents of the aqueous phase, whereas, in the second one, they are structuring agents suitable for producing different materials like emulgels. As expected, the comparison between two systems showed very different rheological and microstructural behaviour even at the same concentration. In the case of suspensions of undenatured system, the increase of proteins content yields a growing dimension of their aggregates, measured thanks to contrast phase microscopy; all suspensions were liquid-like, and the measured viscosity resulted independent of shear rate and well described by a Krieger- Dougherty model. In the case of thermally denatured systems, the increasing protein content took the aggregates to evolve towards a continuous gel network with a fractal behaviour, as showed by Small Amplitude Oscillation Tests. The main aim of the rheological modelling of both systems is the formulation of predictive equations able to relate macroscopic properties and microstructure; this can allow the design of new food products with predictable properties for different uses.

Wednesday 13:40 Virtual / Track 5 FB14

Drying dynamics in complex mixes of dairy proteins

Ming Yu[1], Cécile Le Floch-Fouéré[1], Françoise Boissel[1], Ludovic Pauchard[2], Arnaud Saint-Jalmes[3], Romain Jeantet[1], and Luca Lanotte[1]
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The dairy powders production represents a significant portion of the market related to dairy industry. Controlling powder nutritional properties has become crucial due to the increasing number of end-users. So far, this question has been addressed taking advantage of the empirical experience gained in the last decades. However, a full understanding of the physics governing the droplet-to-particle transition in industrial dryers, which would be decisive for the tight control of the process, is far from being achieved. To this purpose, the single droplet approach has been used to explore the drying dynamics at the lab scale in dairy simplified model systems, such as mixes of the two milk proteins: the whey proteins (WPI), i.e. globular colloids, and the casein micelles (NPC), i.e. deformable sponge-like structures. In this work, we focused on the evaporation in droplets of WPI/NPC suspensions with different protein concentration (cp) and composition (WPI%R). We investigated the formation of the skin at the air-liquid interface and we explored the paradigm linking protein physico-chemical properties to skin rheology and, consequently, to final droplet shape. A general overview of the process was carried out observing droplet profile evolution and evaluating the drying kinetics by mass measurements. A characterization of the skin organization at the colloidal scale was provided by interfacial rheology, using the oscillatory drop method, and scanning electron microscopy. Our outcomes revealed the separate role of WPI and NPC in skin formation. Under certain conditions, we observed WPI segregation on the external part of droplet surface, which significantly affected dry particle shape. Our systematic approach allowed to obtain a phase diagram able to predict dry particle morphology for a wide range of cp and WPI%R. To summarize, our results represent a potential tool for the control of dairy powder characteristics and contribute also to the understanding of the evaporation in polydisperse colloid systems.

Wednesday 14:40 Virtual / Track 5 FB15

Small and large deformation rheology of acid-induced gels from enzymatically cross-linked caseinates

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Microbial transglutaminase (mTGase) catalyses the formation of covalent isopeptide bonds between glutamine and lysine residues of proteins and thereby affects techno-functional properties. This study follows up on previous research, where the molecular properties of cross-linked casein nanoparticles were linked to certain rheological characteristics of acid gels [1], and presents additional insight into physical gel properties.

Caseinate with different ionic milieus was used as model substrate for cross-linking by mTGase and acid-induced gelation. Time-resolved frequency dependency during gelation was measured by multi-wave tests. The storage modulus increased with frequency following a power law relationship, where the exponent was linearly correlated with the phase angle. The frequency dependency of the loss factor could be fitted with a second-order polynomial function, the minimum of which was shifted to lower frequencies with increasing cross-linking extent. Strain sweep experiments showed less pronounced strain hardening behaviour and reduced fracture strains with increasing cross-linking extents, indicating lower flexibility of cross-linked casein nanoparticles and less non-covalent bonds, respectively. The water holding capacities of the gels were

evaluated by centrifugation and showed a good relationship with the fracture properties, suggesting that the serum drainage during centrifugation was also affected by the strain hardening behaviour.

The results provide relevant new aspects on the mechanisms behind the alteration of gelation properties of caseins as caused by mTGase-induced cross-linking.

[1] Raak et al.: Food Hydrocoll 86 (2019) 43-49.

Wednesday 15:00 Virtual / Track 5 FB16

3D printing of a protein/polysaccharide mixed gel system for food applications

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Three-dimensional (3D) food printing enables the fabrication of customized food designs and creative food flavors with personalized and quantified nutrition, i.e. balanced amount of nutrients. However, there is still a lack of fundamental knowledge on the 3D printing of essential food constituents such as mixtures of proteins and polysaccharides. Here, we developed a water-based protein/polysaccharide ink made of of gelatin B (GB) and xanthan gum (XG) for food 3D printing, based on the understanding of their synergetic gelation. A 40-layer 3D scaffold with defined features was successfully printed using 3 wt% GB and 10 wt% XG aqueous solutions. A reasonable agreement was observed between the shear viscosity measured by rotational rheometry and the process-related apparent viscosity of GB/XG solutions obtained from capillary flow analysis. The ink exhibits a shear-thinning behavior with a relatively low power-law index of about 0.15, typical of soft solids such as XG. The effects of $CaCl_2$ addition and post-deposition temperature on flow properties, shape retention and textural properties were investigated. Both Ca^{2+} addition and low temperature increased rheological properties and gel strength, as indicated by the higher complex viscosity and elastic modulus measured in small amplitude oscillatory shear (SAOS). This is further supported by texture profile analysis. However, Ca^{2+} addition resulted in a syneresis effect, probably because it enhances the interactions between GB and XG. This causes a homogeneous shrinkage of the printed scaffold with time, accompanied by a thickness decrease. The findings of this work that relate printability with rheological properties are part of the knowledge required for providing guidelines for 3D printing in functional food processing, such as personalized food for elderly people and for other sensitive population (i.e. children, pregnant women or athletes).

Symposium ER

Experimental methods and rheometry

Organizers: Christian Clasen and Mariana Rodriguez Hakim

Wednesday 13:00 Virtual / Track 6 ER12

Rheological and optical characterization of water-SLES phase diagram

Rosalia Ferraro[1], Gerardino D'Errico[2], Sergio Caserta[1], and Stefano Guido[1]

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Concentrated aqueous solutions of surfactants pastes are widely used in industrial productions. One of the most common anionic surfactants is Sodium Lauryl Ether Sulfate (SLES). SLES-Water can mix in any proportion but, depending on the composition, the fluid can show completely different rheological behavior, ranging from simple Newtonian aqueous solutions up to complex visco-elastic pastes, as consequence of different rearrangement of surfactant molecules. Surfactant molecules at different concentration can assume different morphologies, such as micellar phases (<30%w of SLES), hexagonal liquid crystals (>30%w), cubic structures (~60%w), or lamellar liquid crystals (>60%w). Temperature also plays a key role in the thermodynamic phase diagram. In this work, we investigated the temperature-concentration phase diagram of the SLES-water system coupling rheological characterization with advanced imaging analysis, and microstructural characterization performed by Electron Paramagnetic Resonance (EPR) using suitable molecular probes. Rheological characterization was performed using a stress-controlled rheometer equipped with cone-plate geometries, to study the fluid viscosity and moduli as a function of the surfactant concentration and temperature (in the range 35-72%wt and 25-60°C). Different phases showed differences in viscosity and elasticity of about 6 orders of magnitude. Using Time-lapse microscopy, the dynamic evolution of the phase changes as a function of temperature was also analyzed for sample with different SLES concentrations. Images acquired using crossed polarizers, were analyzed to measure the mean light intensity and identify temperature and concentration ranges of isotropy/anisotropy, defining different phases diagram. EPR results allowed the supramolecular organization of the various phases to be investigated. The Rheological, optical and EPR results have been finally compared to obtain a complete characterization of the phase diagram.

Wednesday 13:20 Virtual / Track 6 ER13

Advances in rheo-optical methods

Jörg Läuger

Anton Paar Germany, Ostfildern, Germany

Simultaneous use of rheological and optical techniques, i.e. of rheo-optical methods, is helpful to gain a better understanding of the dependencies between the microstructure and the mechanical properties of complex fluids. In this paper, new rheo-optical techniques as well as new applications of existing methods are reported. Microscopy and rheo-confocal microscopy provide direct visualization of material under flow. A combination of microscopy techniques with a dual motor rheometer in counter-rotation mode allows the observation of structures at the stagnation line. A rheo polarized imaging techniques called SIPLI (shear induced polarization light imaging) combines a visualization technique with measurements of local stresses through the detection of the birefringence. By employing parallel-plate geometries, different shear rates are present throughout the sample, from a maximum shear rate at edge of the sample to a zero shear rate in the center of the plate. With SIPLI the whole plate is observed and the birefringence can be displayed over the full range of shear rates within one single experiment. Applications include structure alignments and shear induced phase transitions of different materials such as block copolymers, nano-crystalline cellulose, and polymer melts. Spectroscopic techniques such as IR or Raman are used for detecting chemical change during curing reactions or conformational changes during phase transitions. The phase transition from the crystalline to liquid state for different polymers was monitored by rheo-Raman spectroscopy. Special emphasis has been given to an accurate temperature control over a large temperature range in order to take full advantage of the potential of the various rheo-optical techniques.

Wednesday 13:40 Virtual / Track 6 ER14

Echo-Differential Dynamic Microscopy enables a multi-scale characterization of the microscopic dynamics during non-linear oscillatory rheology experiments

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Oscillatory shear tests are widely used to characterize the linear mechanical response of complex fluids, as they allow to impose a sinusoidal perturbation with variable yet controlled amplitude and frequency. However, the interpretation of the results of oscillatory tests in the non-linear regime remains challenging and somehow ambiguous [1], also but not exclusively because of shear banding [2]. Stimulated by recent work [3], we introduce echo-DDM i.e. Differential Dynamic Microscopy [4] with an echo protocol [5] to obtain an all-optical characterization of the microscopic dynamics of periodically sheared complex fluids: a strain-controlled shear cell mounted on an optical bright-field microscope is used to oscillatory perturb a variety of samples ranging from Hookean solids to yield stress fluids. We first exploit the finite depth-of-focus of the microscope to obtain a complete characterization of the mesoscopic deformation field (wall slip, shear band, time evolution) of the sample. We then use echo-DDM to characterize the microscopic, irreversible rearrangements induced by the external perturbation. We find that complex fluids with different mechanical responses present different types of irreversible shear-induced microscopic dynamics. The proposed methodology is not based on particle tracking, is highly user-independent and can be used with virtually any source of contrast, both using transparent media, seeded with colloidal particles, or using the signal scattered by the material itself; it is applicable to a wide variety of samples and encompasses a large range of length scales, from the particle size to macroscopic ones, providing a promising tool for the exploration of non-linear rheology world.

[1] K. Hyun, et al. Prog Polym Sci 36, 1697-1753 (2011). [2] T. Divoux, et al. Phys Rev Lett 104, 208301 (2010). [3] S. Aime, L. Cipelletti. Soft Matter 12.2 213-226 (2019). [4] R. Cerbino, V. Trappe. Phys Rev Lett 100, 188102 (2008). [5] P. Hébraud, et al. Phys Rev Lett 78.24, 4657 (1997).

Wednesday 14:40 Virtual / Track 6 ER15

Imaging strongly confined flow: a new rheo-MRI setup for probing cooperativity effects

Klaudia W. Milc[1], Maria R. Serial[1], John Philippi[1], Joshua A. Dijksman[2], John P. van Duynhoven[3], and Camilla Terenzi[1]

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Strongly confined flow of complex fluids is encountered in many industrial and everyday-life situations. For instance, in the production of foods or cosmetics, fluids are extruded through mm-sized nozzles into molds, often at elevated temperatures (~20-80 °C), while during customer use the products are spread into µm-thin layers, at temperatures 20-40 °C. The prediction of flow in such varying confinement sizes and temperatures is particularly difficult for structured dispersions, such as thixotropic colloids or concentrated emulsions, whose inter-particle interactions give rise to flow cooperativity under strong confinement. Flow cooperativity results in an enhanced, spatially-heterogeneous fluidization of the material. However, the nature of such flow instabilities still remains not well understood due to both its complex phenomenology and the lack of experimental techniques suitable for studying strongly confined flow of optically-opaque, structured fluids. With rheo-Magnetic Resonance Imaging (rheo-MRI) velocimetry it is possible to measure flow in a spatially-resolved, non-invasive manner even in optically-opaque materials. In this work we present the design of a novel 500 µm gap rheo-MRI Couette cell, which imposes stable flow conditions thanks to the excellent mechanical stability of the bob, and can operate at 15-40 °C. We demonstrate the use of the cell for characterizing flow cooperativity effects in a fat crystal dispersion (FCD), a common food precursor, prepared under varying crystallization rates. The high MRI resolution of our data (~10 µm) enables us to quantify the decrease in cooperativity length of FCDs as a function of cooling rate. As demonstrated with this food precursor,

and in principle applicable to all other optically-opaque structured fluids, our setup can become a useful tool for fundamental studies of flow cooperativity and for deciding on the optimal production conditions.

Wednesday 15:00 Virtual / Track 6 ER16

Coupling reflection polariscope and cone-partitioned plate experiments to investigate shear-induced structural changes in rod-like polymers

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Among the vast realm of polymeric systems, rod-like polymers display the unique feature of forming ordered mesophases, i.e. nematic phases. In the simplest case, the nematic phase manifests either within only a certain temperature range (thermotropic nematics), or within a specific range of temperature and concentration (lyotropic nematics). Interestingly, ordered structures can also be promoted by shear flow. In such a case the boundaries to form a nematic phase are controlled by the shear flow, or more specifically, bv the minimum shear rate needed to align and stretch the rod-like polymers towards the flow direction, enabling the possibility to form nematic domains. Typical signatures of a nematic phase reflect on the presence of significant shear-induced birefringence, as well as on the shear rate dependence of the steady-state viscosity. However, measuring reliably the steady-state viscosity with rotational rheometers is not trivial, and most of the times flow instabilities manifest as a perturbation of the material at the gas/sample interface; known as edge fracture. Here we propose the combination of two independent techniques which provide quantitative optical and rheological information: 1) A reflection polariscope installed in a Physica MCR-502 Anton Paar rotational rheometer, for shear-induced birefringence measurements, and 2) a home-made Cone-Partitioned Plate installed in a TA Instruments Ares-G2 rotational rheometer, for shear viscosity and first normal stress difference measurements, unaffected by edge fracture. Such a combination allows us to estimate the stress-optical coefficient of rod-like polymers, and obtain extended and reliable flow curves, necessary ingredients for polymer processing and modelling.

Symposium CF

Complex flows

Organizers: Rossana Pasquino and Francisco Galindo Rosales

Wednesday 13:00 Virtual / Track 7 CF3

Sedimentation of triaxial ellipsoidal particles in a viscoelastic fluid

Gaetano D'Avino
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Sedimentation of rigid particles immersed in a viscoelastic liquid occurs in a variety of industrial applications. The falling dynamics and the terminal velocity attained by the particle depends on the magnitude of the applied force, the particle shape and size, and the rheological properties of the suspending fluid. The settling of spherical particles in viscoelastic fluids has been thoroughly investigated. In contrast, only few numerical and experimental studies are available for particles with anisotropic shapes, limited to axisymmetric geometries (e.g., cylinders or spheroids) and mainly focused on the final orientation attained by the particle. In this work, we carry out 3D finite element simulations to study the dynamics of a rigid particle with triaxial ellipsoidal shape immersed in an unbounded viscoelastic fluid and subjected to a constant force. An Arbitrary Lagrangian-Eulerian formulation is adopted to handle the particle motion. The orientation dynamics and the resulting drag correction coefficient are investigated. The effect of the Weissenberg number, particle aspect ratios (including oblate and prolate spheroids), and fluid shear-thinning is studied. The flow and stress fields around the particle are also inspected in order to evaluate the possible formation of a negative wake behind the particle and its relation with shape anisotropy.

Wednesday 13:20 Virtual / Track 7 CF4

Bubble alignments in concentrated emulsions in shear flow

Blandine Feneuil, Andreas Carlson, and Atle Jensen
University of Oslo, Oslo, Norway

Formation of particle chains in viscoelastic fluids in simple shear has been first reported in [Michele et al. Rheol. Acta 16, 317-321 (1997)]. Later, experimental studies and simulations have been performed to quantify the role of the fluid rheological properties, namely normal stress differences and shear thinning, on particle chaining. We report experiments exhibiting a similar behavior for bubbles suspended in a concentrated emulsion in a Couette cell. First, we study more than 100 bubbles initially randomly distributed in the cell, and investigate the effect of the bubble size, emulsion rheological properties and shear rate. We obtain after shearing two final bubbles configurations, both with bubbles aligned in the direction of the flow: bubbles in chains, i.e. close to each other, and separation distance several times the bubble diameter. In addition, we note that chaining velocity scales with the strain, in accordance with previous observations on particles. Additional experiments on bubble pairs shows that depending on their relative initial position, two bubbles can either attract or repel each other.

Wednesday 13:40 Virtual / Track 7 CF5

Active control of jet breakup and droplet formation using temperature modulation

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Prilling, a widely used method for production of fertilizers and polymers, is an industrial scale process involving break-up of non-Newtonian molten jets followed by their consecutive crystallization. From a fluid mechanics and rheology point of view, the challenge is to control the drop formation of a slender jet with rotational body forces, non-Newtonian effects and heat transfer. In this numerical study, we focus on the heat transfer ignoring the non-Newtonian effects, more specifically we explored the possibility of using thermal modulation at the nozzle to control the breakup phenomena. Controlling drop formation is of interest beyond prilling. Continuous ink jet printing, a widely encountered process, is such an example where controlling drop formation is relevant. The main perturbation mechanisms to achieve breakup control have so far been the mechanical perturbations which either modulate the pressure, velocity or the size of the orifice, all of which introduce a local curvature that grows convectively. The appeal for thermal modulation, the focus of this study, is the elimination of moving parts in a large-scale system such as prilling. Moreover, the underlying physics of thermally triggered instability remains underexplored. Our results show that temperature modulation does lead to instability through capillary and Marangoni stresses, providing a better control of the droplet formation at the tip of the jet stream which is otherwise irregular. Convective growth of the stresses point out that when the temperature sensitivity of surface tension is low, the growth of the capillary stress is similar to the mechanically perturbed jets. At higher sensitivities, the fluctuations in Marangoni stress dominate the process. More downstream, they go out of phase and start to counteract each other, hence inhibiting the growth. This sets a limit to the shortest breakup lengths achievable by this method of perturbation.

Wednesday 14:40 Virtual / Track 7 CF6

Flow and stability of a viscoelastic liquid curtain

Antoine Gaillard[1], Matthieu Roché[2], Sandra Lerouge[2], Cyprien Gay[2], and Laurent Limat[2]
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The flow and the stability of viscoelastic liquid curtains are investigated using solutions of flexible and semi-rigid polymer chains. Liquids are extruded from a slot at constant flow rate and fall in ambient air under gravity in the form of rectangular sheets. We show that the flow is characterised by an initial balance between gravity and the elastic stresses arising from the stretching of polymer molecules until inertia finally dominates and the classical free-fall behaviour is recovered. The curtain dynamics is mostly influenced by the value of the extensional relaxation time of the solution measured by a filament thinning technique. A master curve of the flow is found by analogy with the Newtonian case. Concerning the stability of the sheet, we find that polymer addition stabilises the curtain by preventing hole formation. More interestingly, we observe the onset of a flow instability for the most shear-thinning solutions, where thick bands are formed within the curtain. Visualisations of the flow inside the die reveal that this phenomenon is linked to a flow instability at the contraction plane upstream of the slot where the flow is unsteady and three-dimensional in nature.

Wednesday 15:00 Virtual / Track 7 CF7

Dynamics of Freely Suspended Drops Translating through Miscible Environments

Endre Joachim Mossige, Vinny Chandran Suja, Daniel J. Walls, and Gerald G. Fuller
Stanford University, Stanford, CA, United States

Our work focuses on an experimental investigation of droplets freely rising through a miscible, more viscous liquid. We report observations of water droplets rising through glycerol and corn syrup, which are common household ingredients. Immediately after the drops are formed, they take on prolate shapes and rise with constant velocity without expanding in size. However, after a critical time predicted by our theory, the drops continually grow into oblate spheroids, and as they mix with the ambient liquid, their volume increases and their velocity decreases, eventually following power laws. We present scaling relations that explain the main observed phenomena. However, the power laws governing the rate of the volumetric increase and the velocity decrease, namely time to the one half and time to the minus one half power, respectively, remain points of further investigation.

Symposium FI

Flow instabilities

Organizers: Sandra Lerouge and Mahdi Davoodi

Wednesday 13:00 Virtual / Track 8 FI12

The onset of purely elastic and thermo-elastic instabilities in Taylor-Couette flow as a function of gap ratio and fluid thermal sensitivity

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Linear stability analysis of Taylor-Couette flow of dilute polymeric solutions has been performed by using two prototypical constitutive equations for polymeric solutions, namely, the Oldroyd-B and the FENE-P models. The hydrodynamic stability characteristics of the flow in the presence and absence of thermal effects and in the limit of vanishing fluid inertia have been determined using an eigenvalue analysis. Particular attention has been paid to accurately determine the instability onset conditions as a function of fluid thermal sensitivity and gap ratio. We observed a reduction in the critical Weissenberg, Wic, for the instability onset as the gap ratio and fluid thermal sensitivity are enhanced. In particular, under non-isothermal conditions, Wic was reduced by almost an order of magnitude for all gap ratios. Our results suggest that the experiments leading to observations of "purely elastic turbulence" in the Taylor-Couette flow at order (1) Wi by Groisman and Steinberg (2004) [1] were not performed under isothermal conditions. Hence, this new flow state should be labeled "thermo-elastic turbulence".

Wednesday 13:20 Virtual / Track 8 FI13

On the influence of particle migration on flow transitions of a suspension Taylor-Couette flow

Lina Baroudi[1], Madhu V. Majji[2], and Jeffrey F. Morris[3]

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In this study, we present an experimental investigation into the effect of inertial migration of particles on flow transitions of a suspension in Taylor-Couette geometry with a stationary outer cylinder and rotating inner cylinder. This work considers primarily transitions associated with the circular Couette flow (CCF) and Taylor vortex flow (TVF) regimes for a suspension of neutrally buoyant particles of size d_p=230 μm at a concentration of φ=0.10. A flow structure (CCF or TVF) near the transition boundary with either uniform particle distribution across the annular region or fully migrated concentration profile is established. The Reynolds number (Re) is subjected to a rapid step change to study the effect of the concentration profile on the flow transition Re and resulting flow structure evolution. Our results show that, relative to uniform concentration, the particle distribution following inertial migration destabilizes the CCF state near the CCF-nonaxisymmetric flow transition boundary. In contrast to this destabilizing effect in CCF, migration of particles in the TVF regime has a stabilizing effect on the TVF-wavy Taylor vortex and TVF-nonaxisymmetric flow transition boundaries. The transition away from the TVF exhibits hysteresis associated with migration, as once initiated TVF could be sustained below and above the transition boundaries observed for suspension TC flow with uniform concentration. Clear evidence of the role of inertial migration and the resulting nonuniform particle fraction in the hysteretic behavior is established by our work.

Wednesday 13:40 Virtual / Track 8 FI14

Linearized dynamics and transient shear banding in viscoelastic shear start-up flows

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We use the Johnson-Segalman and non-stretching Rolie-Poly models to analyze transient dynamics of viscoelastic flows, with a specific focus on the existence of signatures of transient shear banding during start-up shear flow between two parallel plates. We explore the dynamics of shear start-up flow in both monotonic and non-monotonic regions of the constitutive curves of these models using two different methodologies: (i) a 'frozen-time' linear stability analysis, wherein we examine whether infinitesimal perturbations imposed on instantaneous stress components (treated as quasi-steady states) exhibit exponential growth, and (ii) a numerical solution of the linearized governing equations, wherein the linearized perturbations co-evolve with the start-up shear flow. We explore the connections between the results from these two different methodologies and determine whether pronounced transient shear banding is present in the above constitutive models.

Wednesday 14:40 Virtual / Track 8 FI15

Anomalous rheological response of nematic platelets studied by 3D Rheo-SAXS and XPCS

Pavlik Lettinga

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Dispersions of colloidal Gibbsite platelets in the nematic phase show intriguing anomalous behaviour when sheared, due to the strong wall anchoring of such systems. When subjecting this system to Large Amplitude Oscillatory Shear, an elastic response is observed at low strain

amplitudes, but time-resolved rheo-SAXS experiments show that the structural response is symmetry broken. At high strain amplitude a yielding transition between elastic and plastic deformation is observed during a period, accompanied by a flipping of the director. When applying Large Amplitude Oscillatory Stress, the system displays a strong offsets in the rheological response as well as asymmetrical behavior in the microscopic structural response. With increasing stress amplitude the offset of the rheological response diminishes and the microscopic response becomes more symmetric. However, this strongly depends on the frequency of the stress input, and hence the time necessary for the system to yield. Here we tracked the full 3D rotational motion of the director by employing plate-plate and concentric cylinder Couette geometries as well as a vertical X-ray beam. Finally, we show that the response throughout the gap is strongly inhomogeneous, as well in structure as in velocity. To this end we performed XPCS measurements in "tangential" scattering geometry in a Couette cell to obtain velocity profiles.

Symposium MP

Multiphase and other complex fluids

Organizers: Mario Minale and Dganit Danino

Wednesday 13:00 Virtual / Track 9 MP12

Viscoelasticty and dye absorption of graphene oxide based composite hydrogels

Alain Ponton, Yu Lei, Imane Boucenna, and Véronique Thévenet
Faculté des Sciences, Université de Paris et CNRS, Paris, France

Graphene, a new kind of single-layer and two-dimension carbon material, has been widely investigated due to its excellent electrical conductivity, thermal stability, mechanical property and adsorption ability giving rise to many applications. However, the dispersion of graphene is extremely low. Graphene oxide (GO), a precursor for graphene, possesses abundant negatively charged oxygen functional groups such as hydroxyl, epoxy, carboxyl on their basal planes and edges, leading to the good dispersion and the stable colloidal suspension in water or organic solvents. Meanwhile, these oxygen-containing groups make it possible to have strong interactions between polymer and GO to prepare GO-based composites. This study highlights the elaboration of composite hydrogels by introducing aqueous GO dispersion in PVA (polyvinyl alcohol) hydrogels prepared by repeated freezing and thawing cycles without adding crosslinker. The effects of initial concentration of PVA and GO and the number of freezing-thawing cycles on the rheological properties and adsorption behavior of PVA/GO composites were investigated. An improvement in viscoelastic property of PVA/GO composites is observed with the increase of PVA, GO concentration and number of freezing-thawing cycles. Cationic dye methylene blue (MB) adsorption revealed that the adsorption process for PVA/GO composites is mainly enhanced by increasing GO concentration. An attempt is proposed to discuss viscoelastic properties and adsorption capacity in relation with microstructure demonstrating the interest of these composite hydrogels as effective absorbents.

Wednesday 13:20 Virtual / Track 9 MP13

Effect of the cellulose degree of substitution on the phase separation and gel formation of HPMC solutions

Saray Perez Robles, Claudia Carotenuto, and Mario Minale
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Thermoreversible hydrogels are polymer aqueous solutions that reversibly transform into a gel upon temperature changes. Among the natural polymers that exhibit sol-gel behavior, cellulose derivatives have plenty of applications due to their properties of tightening up and shape memory, film formation and barrier skills, and boil-out and bursting avoidance at high temperatures. Many applications are performed in food, cosmetic, medical, pharmaceutical, and oil and gas industries. Some of the polymers that exhibit inverse thermogelation are methylcellulose (MC), hydroxypropyl cellulose (HPC), and hydroxypropyl methylcellulose (HPMC). Their chemical structure is made of a cellulose chain with methoxy or hydroxypropyl substitutions, whose quantities attribute partial hydrophobicity and particular characteristics to each polymer. For HPMC hydrogels, dynamic rheological measurements during heating have shown a smooth decrease of the storage (G') and loss moduli (G") up to T1, followed by an abrupt fall until T2 and a subsequent increase of G' over G" until the final gel strength is reached. Among the hypotheses to explain inverse thermogelation, the most popular suggests that physical intermolecular associations of hydrophobic functional groups occurred due to dehydration. However, most recent studies on MC and HPMC confirmed phase separation and fibrils formation during the heating ramp, explaining the moduli behavior. The HPMC partial phase separation observed while increasing the temperature leads to polymer-rich aggregates suspended in a polymer-poor matrix; subsequently, from the rich phase, the polymer forms fibrils that will associate to build the gel. In this regard, the objective of this work is to understand the effect of the degree of substitution, molar substitution, and molecular weight during the nonequilibrium phases. Rheological evaluations of the heating and cooling cycles of the hydrogel using different geometries, and at different concentrations were done using three different HPMC samples.

Wednesday 13:40 Virtual / Track 9 MP14

Effect of confinement on tube flow of Carbopol in water

Raffaele Graziano[1], Valentina Preziosi[1], Behzad Mohebbi[2], Jan Claussen[2], Giovanna Tomaiuolo[1], and Stefano Guido[1]

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Carbopol, a high-molecular weight homo-polymer of acrylic acid intramolecularly cross-linked by polyethers, is a widely used thickener in many industrial applications, from personal care to drug delivery. Once dissolved and neutralized in water, Carbopol exhibits a yield stress at rather low concentrations, which can be ascribed to the interactions among swollen polymer particles. The latter have been recently imaged by confocal microscopy and fluorescent labeling. By separating particle aggregates from the continuous phase through centrifugation, we have also provided evidence of a miscibility gap in the phase behavior of Carbopol in water. Here, we extend such previous work by investigating confined tube flow of Carbopol in water as a function of flow rate, tube radius and polymer concentration. Particle tracking was used to determine the velocity profiles under different experimental conditions. A velocity plateau was found in a plug core, which was followed by a steep velocity gradient near the wall. The size of the plug core was strongly dependent on flow, geometrical and composition parameters. The swollen Carbopol particles were concentrated in the plug core and close to the wall, with a particle-depleted zone in between. Velocity profile and rheometric data are compared and discussed in terms of the heterogeneous distribution of Carbopol particles along the tube radius.

Wednesday 14:40 Virtual / Track 9 MP15

Normal stresses at the yielding point

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Normal stresses are found in most complex fluids, and yield stress materials are ubiquitous in nature and industries. These facts are the motivation of the present research, which aims to study normal stresses developed in shear flow for different yield stress materials, specifically a Carbopol dispersion, a commecial hair gel, and a highly concentrated emulsion. The goal is to analyze the stress state required to cause yielding in yield stress materials when a shear load is imposed. A simple but efficient experimental protocol is introduced, using a commercial strain-controlled rheometer to measure the normal stresses while the fluid undergoes steady and transient shear rheological tests. Furthermore, the validity of the Von Mises criterion is checked for the materials tested in this study. The results of this study allow, for shear flow, the determination of the yield stress tensor, that is the stress tensor at the yielding point. It was observed that the initial state plays an important role in the normal stresses. Residual stresses were found to be responsible for the difficulty in reaching repetitive measurements. At low shear rates, values of normal stresses substantially higher than the shear yield stress are observed, for all yield stress materials investigated. In addition, for one of these materials, the measured normal stresses go from positive to negative values as the shear stress is varied from above to below the yield stress. The normal stress values for the Carpobol dispersion tested remained constant at low shear rates. Among other findings, it is observed that the time needed to reach a steady state is much longer for normal stresses than for the shear stress, as already stablished in the literature for polymeric liquids.

Wednesday 15:00 Virtual / Track 9 MP16

Shear-controlled acceleration of slow phase transitions in diblock polymer liquid crystals

Connor S. Valentine and Lynn M. Walker

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Low molecular weight, amphiphilic diblock copolymers in selective solvent exhibit complex phase behavior and macroscopic properties that affect the processing and application of these materials. The amphiphilic nature of the diblock copolymer molecules drives assembly of micelles. For a given polymer architecture, concentration, temperature, and solvent quality, micelles will form crystalline lattices known as lyotropic liquid crystals (LLCs). The mechanical properties of these concentrated solutions arise from the crystalline structures and sample history.

Here we use SAXS data taken at the APS at Argonne National Lab to study the impact of oscillatory shear on the micellar crystal structures seen in Brij-58 (C16E20). This system has multiple accessible LLC packings including body-centered cubic (BCC), face-centered cubic (FCC), hexagonally close-packed cylinders (Hl), Frank-Kasper Sigma (s), and Frank-Kasper A15 (A15) [1]. We initiate a metastable BCC packing, by rapidly cooling from the Hl state. Under static conditions, the subsequent transition to the equilibrium A15 phase occurs over the span of 5 months. We show that oscillatory shear can be used to adjust this timescale to achieve the equilibrium state in a matter of minutes. The effect of amplitude and frequency on this timescale is discussed. To the best of my knowledge, this is the first demonstration of shear processing to drive the transition to equilibrium structures in block copolymer melts or solutions.

The phase changes in concentrated block polymer solutions can be quite rapid, or take place over the span of months. These structural changes can be accompanied by drastic changes in material properties. This presents unique challenges during small and large scale processing, as a well behaved liquid mixture can suddenly become an immovable glass within minutes. We aim to understand how processing these materials with shear flows affects these phases and phase transitions

Symposium PG

Powder rheology, granular flows and rheology of solids

Organizers: Alexandra Aulova and Stefan Gstöhl

Wednesday 13:00 Virtual / Track 10 PG12

Comparative analysis of the yield stress and thixotropy of injection grouts for masonry consolidation

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Stone masonry is a constructive technique that has been extensively used in the past due to its simplicity and, consequently, it is present in many ordinary and historic buildings across Europe. The performance of stone masonry walls relies on their monolithic behavior rather than on the mechanical properties of its individual elements. For this reason, masonry walls often need consolidation to improve mechanical performance, such as adhesion between elements and load bearing capacity. Grout injection is a frequently used technique for the consolidation and strengthening of old stone masonry walls. Grouts are concentrated suspensions that can be seen as mixtures of binder with water. To ensure an adequate flow of the grout inside the masonry, it is essential to control the rheological properties of grouts. Previous studies have shown that cementitious-based grouts can be assimilated to yield stress fluids. Yield stress indicate the critical stress value at which the grout will start or stop flowing, which is relevant for the design of grouting operations. Despite the relevance of yield stress for injection grouts, the yield stress is often determined as an isolated parameter without considering phenomena such as thixotropy and hydration. In this study, the determination of yield stress of natural hydraulic lime-based grouts was performed with different measurements methods using a rotational rheometer. The change in yield stress with time due to hydration was determined. Two yield stress, static and dynamic, and the critical shear rate were also measured, which can be used in the grouts design in order to achieve better grouting performance.

Wednesday 13:20 Virtual / Track 10 PG13

Measurements of rheological properties of hydrate slurry formed in water-based drilling fluids

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While drilling in deep water, gas hydrates may be formed when light compounds from the reservoir flow into the wellbore as a result of a kick. To restart drilling fluid circulation, the hydrate crystalline structure must be broken to remove the hydrate slurry from the system. Although important, there is a lack of information about the rheological properties of hydrate slurries formed in drilling fluids. To investigate the rheological properties, hydrate formation was induced by adding tetrahydrofuran (THF) to water-based drilling fluid, allowing hydrate crystallization at atmospheric pressure. The structure formed is an sII type that is found in many hydrates formed with natural gas in oil and gas fields. The rheometric results show that the formed hydrate slurry is a time-dependent elastoviscoplastic material in which the microstructure is irreversibly affected by shear. The influence of shear during the hydrate formation was analyzed and the results showed that the elastic modulus and the yield stress of the hydrate slurry obtained in static formation were more than one order of magnitude larger than those measured in dynamic (imposing shear) formation. Finally, the material showed a brittle solid-like structure in which mechanical response variations are observed at a very low oscillation strain (in the order of 10-3 %).

Wednesday 14:40 Virtual / Track 10 PG15

Superdiffusive microscopic dynamics govern non-Maxwellian stress relaxations in arrested associative hydrogels

Jake Song[1], Qingteng Zhang[2], Felipe de Quesada[1], Marc Piquette[3], Mehedi H. Rizvi[4], Joseph B. Tracy[4], Emanuela Del Gado[5], Suresh Narayanan[2], Niels Holten-Andersen[1], and Gareth H. McKinley[1]
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We investigate the microscopic dynamics of a deeply arrested associative hydrogel system using x-ray photon correlation spectroscopy (XPCS). This system consists of metal-coordinating catecholic telechelic polymers, which begin from an equilibrium state and - through multi-functional reversible cross-linking with iron oxide nanoparticles - are equilibrated into a deeply arrested gel state. This arrested state manifests in the form of non-Maxwellian stress relaxations, characterized by a broad spectrum of relaxation modes in a stretched exponential or power-law manner. Our investigation shows that these hydrogels exhibit hallmark behaviors of arrested systems such as compressed exponential relaxations, superdiffusive dynamics, and quantifiable fluctuations in higher-order correlations indicative of dynamic heterogeneity. Although these observations are often associated with non-equilibrium dynamics, we nevertheless find that this system exhibits hallmark equilibrium behaviors, as demonstrated by an absence of static and dynamic aging effects, and by the Gaussian distributions of relevant fluctuation quantities such as the instantaneous fluctuations at different delay times and the relaxation times. The relationship between superdiffusive microscopic dynamics and non-Maxwellian macroscopic stress relaxations in this system are explored directly through temperature-dependent correlation studies; these studies demonstrate that the superdiffusive microscopic relaxations follow Arrhenius scaling, and that this apparent activation energy at the microscale accurately describes the temperature-dependency of the macroscopic stress relaxation data. Moreover, we demonstrate that a direct estimation of the power-law exponent of the stress relaxation from the scaling exponent that quantifies the superdiffusive dynamics, following recent computational work by Riggleman and Crocker (DOI: 10.1038/nmat4663), is possible and yields an excellent agreement with the stress relaxation data.

Wednesday 15:00 Virtual / Track 10 PG16

Impact of delayed elastic storage on the slow viscoelastic response of foams

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Liquid foams are soft jammed materials that constantly reconfigure due to coarsening-induced intermittent bubble rearrangements. Thus, while elastic at short time, the long-time response of a foam to a small stress is similar to that of a normal viscous fluid, namely the strain increases linearly in time. Although such fluid response generally entails an exponential stress relaxation when a small strain is applied, our measurements reveal a much more complex behaviour. Here, we show that such complexity relates to a process of gradual elastic storage evidenced in creep-recovery experiments. We show that these delayed elastic effects also contribute to the low frequency behaviour in oscillatory strain experiments.

Symposium MN

Micro and nano fluidics and microrheology

Organizers: Anke Lindner and Laura Casanellas

Wednesday 13:00 Virtual / Track 11 MN12

Yielding of a Carbopol gel in a confined microscopic flow: fluid dynamics, solid mechanics or ... else?

Eliane Younes[1], Michal Himl[2], Zdenek Stary[3], and Teo Burghelea[1]
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In spite of a continuously increasing number of studies, the physics of yielding of a physical gel in a confined microscopic flow remains elusive. Recent attempts of understanding the dynamics of the solid-fluid transition rely on micro-structural phenomenological pictures involving a scalar function (generally referred to as structural parameter) that combine ideas from both the fluid dynamics and solid mechanics communities. Recently, it was suggested that statistical physics and critical phenomena provide useful insights into solving the "yielding puzzle", [1,2] . Through this contribution, we test for the very first time these ideas by means of in-situ visualisation of flows and micro-structure of a Carbopol gel in a plane micro-channel flow. By means of a novel chemical protocol able to stain the solid material units of the gel with a fluorescent molecule we are able to accurately identify the solid/fluid material units advected by the confined microscopic flow. Based on this novel visualisation technique a full statistical description of the distributions of solid-fluid material units in the flow in terms of space and time averages, probability density functions and space-time correlations is reported for the first time. We finally conclude that the most appropriate description of the microscopic yielding process of a viscoplastic material needs to be made in terms of statistical quantities rather than in a deterministic manner.

[1] R. Sainudiin, M. Moyers-Gonzalez, and T. Burghelea A Microscopic Gibbs field model for the macroscopic yielding behavior of a viscoplastic fluid, Soft Matter, 11, 5531-5545, 2015.
[2] T. Burghelea M. Moyers-Gonzalez and R. Sainudiin, A nonlinear dynamical system ap- proach for the yielding behaviour of a viscoplastic fluid, Soft Matter, 13, 20204-2039, 2017.

Wednesday 13:20 Virtual / Track 11 MN13

Yield stress in a flash: investigation of nonlinearity and yielding in soft materials with an optofluidic microrheometer

Valerio Vitali[1], Giovanni Nava[2], Andrea Corno[2], Melissa Pezzotti[1], Francesca Bragheri[3], Petra Paiè[3], Roberto Osellame[3], Marco Aldo Ortenzi[4], Ilaria Cristiani[1], Paolo Minzioni[1], Tommaso Bellini[2], and Giuliano Zanchetta[2]
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Yield stress fluids (found in food, biological networks, cosmetics) deform as elastic solids or flow as viscous liquids, depending on whether the stress applied upon them is below or above a threshold value [1]. This dual behaviour is also at the basis of their ability to trap particles below a certain size or density, while being easily poured, with widespread application in personal care products. However, the origin and conditions of such a transition display several open issues, like the stress distribution within the material or the role of microstructural dynamics. We can directly elucidate the yielding mechanisms by comparing macro- and micro-scale mechanical properties, e.g. with tools like optical

tweezers, which are however limited in terms of attainable forces and are thus often insufficient to induce local failure. We demonstrate that a recently developed microrheology setup, based on a optofluidic chip and optical scattering forces acting on a microbead [2,3], is ideally suited for yield stress measurements, thanks to the fine control over applied forces up to 1 nN, thus providing access to a wide range of phenomena. We perform creep and recovery experiments on an aqueous suspension of packed, swollen microgels. From the different regimes observed in the motion of the microbead, linear and yielding properties of the material are readily estimated. We find good agreement with bulk rheology measurements. However, the details of microbead trajectory offer some hints on the microscopic mechanism of yielding: both at low and high forces, it advances in a series of small yielding events corresponding to intermittent or periodic microgel rearrangements within the material. Furthermore, small passive tracers allow us to estimate the extent of the fluidized region around the microbead, which agrees with previous estimates for large particles.

[1] D. Bonn et al., Rev.Mod.Phys., 89, 035005 (2017). [2] G. Nava et al., Soft Matter, 14, 3288 (2018). [3] V. Vitali et al., Sci.Rep., 10, 1 (2020).

Symposium NF

Living and self-assembling systems

Organizers: Daphne Weihs and Jan Vermant

Wednesday 14:40 Virtual / Track 11 NF1

Fluctuations enhance particle clearance in the respiratory system

Arnold J. Mathijssen

Physics and Astronomy, University of Pennsylvania, Philadelphia, PA, United States

Our airways are continuously exposed to potentially harmful particles like dust and viruses. The first line of defence against these pathogens is a network of millions of cilia, whip-like organelles that pump flows by beating over a thousand times per minute. In this talk, I will discuss the connection between local cilia architecture and the topology of the flows they generate. We image the mouse airway from the sub-cellular (nm) to the organ scales (mm), characterising quantitatively its ciliary arrangement and the resulting flows. Interestingly, we find that disorder in the ciliary alignment can actually be beneficial for this pathogen clearance. More generally, I would also like to discuss how systems can be driven out of equilibrium by such active carpets. Combining techniques from statistical and fluid mechanics, I will demonstrate how we can derive the diffusivity of particles near an active carpet, and how we can generalise Fick's laws to describe their non-equilibrium transport. These results may be used for new self-cleaning materials, much like our airways.

Wednesday 15:00 Virtual / Track 11 NF2

Injectable hydrogel formulations to host adipose stem cell spheroids for stemness maintenance and bone and cartilage regeneration

Emanuela Muscolino[1], Anna Barbara Di Stefano[2], Francesca Toia[2], Maria Antonietta Sabatino[1], Francesco Moschella[2], Adriana Cordova[2], Daniela Giacomazza[3], and Clelia Dispenza[1]

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Adipose-derived mesenchymal stem cells (ASCs) represent a great promise for tissue regeneration as fat is a very abundant source of stem cells and owing to their ability to self-renew and differentiate into specific tissue types. ASCs are usually cultured in 2D, not representative of the in vivo condition. When ASCs are cultured in low adhesion flasks and with a suitable culture medium, they aggregate in the form of three-dimensional spheroids (SASCs). The incorporation of these spheroids into injectable, in-situ gelling, polymer solutions can preserve the 3D structure of the cells from extraction to administration, avoid uncontrolled cell spreading, poor interaction and integration with the surrounding tissue. Moreover, in the presence of the right signaling molecules, SASCs are ready to differentiate in osteogenic and chondrogenic tissue, therefore, incorporated in the right scaffold, they can be very useful to repair both cartilage and bone defects that are still a challenge for modern medicine. As scaffold, hydrogels can meticulously look like the native ECM, due to their interconnected pore architecture, high water content and amenability to incorporate biomolecules or to provide specific biomechanical cues. Therefore, maintenance of stem cell viability and stemess potential, induction of differentiation, support for cell proliferation and spreading with minimally invasive procedures. Our work explores the suitability of hydrogels obtained by temperature-triggered self-assembly of partially degalactosylated xyloglucan aqueous dispersions (dXGaq) as SASCs niches for stemness considtions maintenance or for their differentiation in either osteogenic or chondrogenic lineages. The influence of the different culture media mixed with dXGaq and the presence of SASCs in the mixtures on the flow properties before gelation of all the above and the extrusion process with a syringe on the formed physical networks were investigated by shear viscosity and small amplitude oscillatory rheological analyses.

Symposium CS

Colloids and suspensions

Organizers: George Petekides and Valeria Garbin

Wednesday 13:00 Virtual / Track 12 CS40

Rheo-imaging of cement pastes: shear strain heterogeneities under oscillatory shear

Subhransu Dhar, Teresa Liberto, and Agathe Robisson

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Fresh concrete slurries notoriously exhibit complex behavior under shear, with the formation of lubrication layers attributed to particle migration [1,2]. These lubrication layers are essential to enable the pumping of concrete during civil constructions (i.e. bridges, buildings, oil wells...). However, when such complex suspensions are sheared in a rheometer, the formation of flow heterogeneities introduces errors in properties estimation.

In this work, we apply large strain amplitude oscillations ("pre-shear") to fresh cement pastes under parallel plate geometry. Optical imaging and particle image velocimetry (PIV) are used to measure local shearing deformations on the plate outer radius, while angular deflection and stress amplitudes are simultaneously recorded. The images are analyzed using the MATLAB PIVlab toolbox and velocity profiles are obtained. After the pre-shear, small strain amplitude oscillations are applied and the evolution of the elastic modulus with time is measured ("structuration"). This protocol is applied to several cement pastes with different particle dimensions and comparable yield stresses, which are then varied using a common superplasticizer (PCE).

Our work demonstrates that heterogeneities develop in all samples (on their outer radius) and are more severe for high yield stress pastes. We argue that the appearance of these heterogeneities during the pre-shear phase influences the values and evolution of elastic modulus during the structuration phase, questioning their accuracy.

[1] S. Choi et al. CCR, 2013. [2] A.M. Ley-Hernández and D. Feys, Rheology and Processing of Construction Materials, 2019 (228-236).

Wednesday 13:20 Virtual / Track 12 CS41

Microscopic origin of flow for dense granular suspensions

Romain Mari

LIPhy, Université Grenoble Alpes, CNRS, Grenoble, France

The flow of dense granular suspensions is dominated by the physics of the jamming transition, where the viscosity diverges. At concentrations just below the jamming transition, proliferating contacts considerably limit the number of degrees of freedom left for the particles to move along. In suspensions of frictionless particles, the remaining unconstrained degrees of freedom are highly collective "floppy modes", along which the flow proceeds smoothly. Crucially, the collectiveness of these floppy modes increases when approaching jamming: velocity fluctuations become correlated on a length scale which diverges at jamming. For granular suspensions of frictional particles, however, this scenario has been recently questioned, and numerical simulations suggested some sort of flow heterogeneity based on the measured statistics of contact sliding velocities. In this work I show with Discrete Element simulations that indeed, for some range of friction coefficients, close to jamming the flow does not proceed smoothly along floppy modes, but rather via short-lived system spanning slip planes. In other words, the flow is localized in space and time, in sharp contrast with the floppy mode scenario. The physical picture is that close to jamming, when the contact friction coefficient is close enough to the macroscopic friction coefficient (the ratio between shear stress and particle pressure), it becomes possible for two stacked slabs of the suspension to behave as solid bodies and slip on top of each other. Because the macroscopic friction coefficient at jamming for granular suspensions is around 0.3, which happens to be close to the contact friction coefficient of many materials, this flow mechanism could actually be way more common than flow along floppy modes. On the modelling side, this opens the possibility of mesoscopic descriptions of flow of granular suspensions near jamming based on assemblies of local visco-plastic elements, in analogy to the mesoscopic elasto-plastic models of yield stress materials.

Wednesday 13:40 Virtual / Track 12 CS42

Competing effects of solvent microstructures and electrostatic interactions on the aging dynamics and rheology of aqueous suspensions of a soft colloidal clay

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The influence of solvent microstructure and electrostatic interactions on the microscopic dynamics and rheology of aging colloidal smectite clay suspensions is investigated by performing dynamic light scattering and rheology experiments. Additives that can either induce interparticle electrostatic attractions or alter the ordering of water molecules in an aqueous medium are incorporated in aqueous Laponite R clay suspensions. While the addition of sodium chloride, glucose and potassium chloride accelerates the aging dynamics of the Laponite particles in suspension and leads to rapid dynamical arrest, the presence of N, N-Dimethylformamide is seen to significantly disrupt the aging and jamming dynamics of the particles. When temperature of the solvent is raised, the suspension approaches kinetic arrest more rapidly, indicating the decrease of the Debye screening dominates over the disruption of hydrogen bonds under these conditions. The aging dynamics and rheology of the samples are correlated with their microstructural details visualized using cryogenic electron microscopy. Our data demonstrate that the microscopic dynamics of aging Laponite suspensions show self-similar time-evolution, while their nonlinear rheological responses are sensitive to the temperature of the suspension medium and the presence of additive molecules.

Wednesday 14:40 Virtual / Track 12 CS43

Phenomenological Model of Viscoelasticity for Systems Undergoing Sol-Gel Transition

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A material undergoing sol-gel transition evolves from the pre-gel (sol) state to the post-gel state, through the critical gel state. It is well-known that critical gels exhibit power-law rheology. The faster decay of the relaxation modulus in the pre-gel state can be empirically described by modifying this power-law decay with a stretched exponential factor. A phenomenological analytical expression for the relaxation modulus in the post-gel state is proposed by invoking symmetry associated with the evolution of relaxation time on either side of the critical gel state, and by accounting for natural constraints. This expression, which depends on the extent of crosslinking, can be suitably transformed to obtain analytical expressions for the dynamic moduli and the continuous relaxation time spectrum. Thus, the proposed model facilitates a comprehensive description of viscoelastic evolution from the pre-gel to the post-gel states. It is validated by carrying out experiments on a model colloidal gel-forming system, and by considering other diverse gel-forming systems studied in the literature. After calibrating the parameters of the phenomenological model, it is found to be in excellent agreement with experimental data. Such a well-calibrated phenomenological model can be used to determine any linear viscoelastic response over a wide range of frequencies, and extents of crosslinking encompassing the entire sol-gel transition.

Wednesday 15:00 Virtual / Track 12 CS44

The specific sequence of physical processes that causes the loss modulus overshoot in yield stress fluids

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We gain a deeper understanding of the yielding transition by performing an experimental decomposition of the rheological response of simple yield stress fluids under oscillatory shearing. By iteratively performing recovery tests throughout the period, combining strain- and stress-controlled rheometry, the transience of the recoverable and unrecoverable strains is distinguished, and the solid-like and fluid-like contributions to the material's behavior can be experimentally separated in a time-resolved manner. Distinguishing the recoverable and unrecoverable strains allows for solid-like and fluid-like contributions to G" to be defined, respectively. Both contributions are shown to be significant across the entire amplitude sweep. We specifically show that the increase in the acquisition of strain unrecoverably at intermediate amplitudes is responsible for the overshoot in the loss modulus, which has been referred to as the Payne effect or a Type III response. We show that this behavior is consistent across different classes of yielding materials (e.g. microgels, glasses, associative polymers, filled polymer solutions), suggesting a universality of our observations. Beyond the explanation of the G" overshoot, the time-resolved nature of the experimental strain decomposition leads directly to a novel, fully-experimental paradigm for the understanding of large amplitude oscillatory shear (LAOS) data. We experimentally identify the specific sequence of physical processes that occurs in these materials during LAOS: 1) elastic deformation, 2) rapid, non-instantaneous yielding, and 3) plastic flow. We also show that this sequence of processes is nearly identical to that obtained from the analytical sequence of physical processes framework (SPP), which can therefore adequately capture the non-linear physics of yielding materials via simple measurments.

Thursday Morning

Symposium PL

Plenary Lecture

Thursday 8:00 Virtual / Plenary Lecture PL2

Contributions of elastic storage, plastic and viscous dissipation during flow of soft jammed materials

Véronique Trappe[1] and Marco Caggioni[2]

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For the description of the shear rate dependent stress of yield stress fluids it became custom to use the Herschel-Bulkley model that describes the stress dissipated at a given shear rate as a sum of the yield stress and a power law term characterized by the shear thinning exponent. We find that this exponent strongly depends on the effective range of high shear rate data considered. This not only limits the use of the Herschel-Bulkley model to predict the shear rate dependent stress outside the range explored, but also denotes the lack of physical meaning of the fit parameters used. We propose a Three Component model [1] that describes the shear rate dependent stress of soft jammed materials as a superposition of three contributions, elastic storage, plastic and viscous dissipation. Fits obtained by using this model describe the data as accurately as the Herschel-Bulkley model, and more importantly, they provide physically meaningful fit values that can be explored to understand the main parameters governing shear rate dependent stress dissipation in soft jammed materials.

[1] M. Caggioni, V. Trappe, P. T. Spicer, J. Rheol. 64, 413 (2020)

Symposium CS

Colloids and suspensions

Organizers: George Petekides and Valeria Garbin

Thursday 9:20 Virtual / Track 1 CS17

Adhesive Hertzian contact and friction as the origin of atypical asymptotic scalings in capillary suspensions

Irene Natalia[1], Randy H. Ewoldt[2], and Erin Koos[3]

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We report the most complete experimental evidence to date of non-integer power-law expansions for nonlinear viscoelastic properties [1]. Our observations, made with a capillary suspension [2], falsify the universality of the standard assumption where shear stress nonlinearities arise as amplitude cubed, i.e. $\sigma \sim \gamma_0^3$, in an oscillatory shear test at small amplitudes. In terms of material properties, our measurements require non-integer Taylor expansions about a linear reference state. Furthermore, distinct power law exponents are found for the storage and loss signals. In this work, we conclusively demonstrate that the non-integer scaling is real and not an experimental artefact.

We study the physical origins of the atypical scaling by experimentally surveying a range of compositions of the capillary suspensions and by developing a mathematical model of adhesive Hertzian contact for the particle network stress. Capillary suspensions are solid-liquid-liquid systems with sample-spanning network formed by the strong attractive capillary force between the particles [2]. We find that the non-integer scalings occur at every secondary fluid concentration for two different contact angles. This indicates that the non-integer scalings are related to the underlying microstructure of capillary suspensions. We show that the magnitude of the third harmonic elastic stress scaling $m_{3,\text{elastic}}$ can be traced back to adhesive particle contacts generating elastic stress, which arises from the Hertzian-like contact in combination with the attractive capillary force. The related third harmonic viscous stress scaling $m_{3,\text{viscous}}$ is, therefore, associated with adhesive controlled friction. Our results offer a opportunity to study the importance of the particle bonds and friction in the rheological response under low deformation, instead of just at very high shear rates.

[1] Natalia, Ewoldt, Koos, JoR, 2020. [2] Koos, Willenbacher, Science, 2011.

Thursday 9:40 Virtual / Track 1 CS18

Sol-gel transition of colloidal silica suspension investigated by time-resolved rheometry

Panu Noppari[1], Olli-Ville Laukkanen[2], and Jukka Seppälä[1]
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The objective was to investigate the feasibility of time-resolved rheometry (TRR) to determine the sol-gel transition of colloidal silica suspensions (i.e. silica sols) and study the effects of changing the R-value (molar ratio of water to silica precursor) and the pH of the silica sols. Said parameters are known to impact the condensation rate of silica sols. Tetraethyl orthosilicate (TEOS) was used as the precursor and the hydrolysis of TEOS was carried out in deionized water, at pH 2, using 0.1M hydrochloric acid as a catalyst (i.e. acid catalyzed). The R-value of the sols varied from 10 to 400 (i.e. 15 to 0.8 wt.% silica) and the sols were adjusted to a final pH ranging from 4.5-6.2. The time-resolved rheological measurement consisted of consecutive frequency sweeps ranging from 0.1 to 10 Hz under a controlled strain amplitude of 0.05% and a temperature of 25 °C. The mutation numbers corresponding to the storage and loss modulus were shown to be smaller than 0.1 under all test conditions, confirming the quasi-stability of the measured samples during the experimental time. The transition was observed as a steep rise in the measured storage modulus values and simultaneous visible solidification of the silica sol in a glass vial. The time evolution of the storage modulus was successfully modelled with an Avrami-type equation. The TRR measurements showed that increasing the R-value of the silica sols the transition time increased linearly, whereas increasing the pH decreased the transition time exponentially. Furthermore, the frequency dependences of the storage and loss modulus were investigated before, during and after the transition. After the sol-gel transition the samples elicited properties characteristic of colloidal glass as the loss tangent ($\tan \delta = G''/G'$) decreased with increasing frequency.

Thursday 10:00 Virtual / Track 1 CS19

Delayed Yield and Resolidification in Colloidal gels

Esmaeel Moghimi and George Petekidis
IESL-FORTH and University of Crete, Heraklion 71110, Greece

We examine the macroscopic deformation of a colloidal depletion gel subjected to a step shear stress. Three regimes are identified depending on the magnitude of the applied stress. For stresses below yield stress, the gel undergoes a weak creep in which the bulk deformation growths sublinearly with time similar to crystalline and amorphous solids. For higher stresses, when the bulk deformation exceeds approximately the bond length, the sublinear increase of deformation turns into a superlinear growth of strain which signals the onset of non-linear rearrangements involving some bond breaking and lead to yielding of the gel. However, the long-time creep after such superlinear growth shows two distinct behaviors: under strong stresses, a viscous flow is reached in which the strain increases linearly with time. This indicates a complete yielding and flow of the gel. In stark contrast, for weak stresses, the gel after yielding starts to resolidify. Microscopically, resolidification is concurrent with bond formation and gel coarsening under stress. More homogenous gels that are produced through enhancement of either interparticle attraction strength or strain amplitude of the oscillatory preshear, resolidify gradually over time. In contrast, in gels that are more heterogeneous resolidification occurs abruptly. We also find that heterogenous gels produced by oscillatory preshear at intermediate strain amplitude yield in a two-step process. Finally, the characteristic time for the onset of delayed yielding is found to follow a two-step decrease with increasing stress. This is comprised of an exponential decrease at low stresses, during which bond reformation is decisive and resolidification is detected, and a power law decrease at higher stresses where bond breaking and particle rearrangements dominate.

Thursday 11:00 Virtual / Track 1 CS20

Stress vs. Strain Controlled Shear: Yielding and Relaxation of Concentrated Suspensions

Andreas Pamvouxoglou[1], Andrew B. Schofield[2], George Petekidis[3], and Stefan U. Egelhaaf[1]
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The reduced dynamics of concentrated suspensions results in a significant increase of the viscosity and a slow equilibration, if equilibrium is reached at all. The sample properties hence depend on the sample history. In this contribution we will focus on the rheological properties of concentrated suspensions of colloidal hard spheres consisting of poly(methyl methacrylate) (PMMA) particles in an organic solvent. Volume fractions around the glass transition are studied. We compare the effects of strain and stress control during shear and after cessation of shear.

During the application of shear, the transient behaviour significantly depends on whether the sample is exposed to a constant shear rate or a constant stress. In contrast, as expected the steady-state appears independent of the preparation procedure, as long as yielding occurred and the sample is flowing. After cessation of shear, relaxation is followed under strain rate control and, in a separate experiment, stress control, independent on whether initially a constant shear rate or a constant stress was applied thus including unconventional test sequences. If yielding occurred, relaxation is independent of the kind of control during the application of shear, i.e. whether a constant shear rate or stress was applied, whereas there is some effect of the kind of control during the relaxation, i.e. whether the shear rate or stress is set to zero. This indicates that shear can erase some of the sample's memory.

Thursday 11:20 Virtual / Track 1 CS21

Solid inclusions to stiffen a colloidal gel

Claudia Ferreiro-Córdova[1], Maxime Schneider[2], Chiara Guidolin[2], Sandrine Mariot[2], Olivier Pitois[3], Giuseppe Foffi[2], and Anniina Salonen[2]

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The addition of solid particles to an elastic matrix changes the mechanical properties of the material. The size of the particles has no influence on the mechanical properties, which are controlled by the volume fraction of the added particles. The elastic modulus increases following the Krieger Dougherty model as the particle concentration increases. This description also works well when concentrated emulsions are used as the continuous phase.

However, the addition of inclusions into a weakly elastic emulsion, where the origin of the elasticity is not the packing fraction but attractive interactions and gelling, leads to an increase of the elastic modulus beyond what the KD model predicts. This stiffening is more pronounced as the size of the inclusions decreases close to the size of the emulsion drops. A similar effect can be observed in simulations, where solid inclusions are added into an attractive colloidal gel. As the inclusion size approaches the colloidal scale the elastic modulus increases strongly. We show that the origin of the increased elastic modulus is due to the participation of the small inclusions in the network through two effects, increase of the total volume fraction of solid phase and a restructuring of the gel around the small particles.

Thursday 11:40 Virtual / Track 1 CS22

On the origin of the Cox-Merz rule failure in concentrated Newtonian suspensions

Claudia Carotenuto[1], Raffaella Martone[1], Genta Rexha[2], and Mario Minale[1]

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This work tries to individuate the origin of the Cox-Merz rule failure for Newtonian suspensions that in fact always show a complex viscosity smaller than the steady state one. In literature, it is known that the oscillatory shear flow may induce a microstructural reorganization in Newtonian suspension that depends on the applied strain. Two different mechanisms have been individuated: one arising after a large number of cycles [1] and the other in the first few tenths of cycles [2]. These two mechanisms cannot, however, explain the failure of the Cox Merz rule since typically in dynamic experiments only two or three cycles are executed to measure the complex viscosity.

We here studied in detail the rheological behaviour of a Newtonian suspension in the very first cycles of oscillation by coupling experimental tests, under SAOS and LAOS conditions, and numerical analyses, in the Stokesian dynamics framework. We showed that the complex viscosity first decreases with the applied strain amplitude till a minimum at about $\gamma_0 = 1$ and then it increases again. For $\gamma_0 \leq 1$, both experimental and numerical tests suggest that starting from the first half cycle of the first oscillation the structure rearranges so to redistribute the particles more uniformly and to break the clusters randomly present in the suspension. This sort of structure dilation implies the progressive reduction of the measured complex viscosity during the very first cycles of oscillation. For $\gamma_0 > 1$, the oscillatory flow resembles a flow reversal, the larger the strain amplitude the better the similarity, and the final microstructure tends back to the steady one and thus the complex viscosity accordingly increases.

[1] JM Bricker and JE Butler, J. Rheol. 51:735, 2007
[2] Park et al., Phys. Fluids 23:013302, 2011

Symposium PM

Polymer melts and composites

Organizers: Maria Theresa Cidade and Juan de Vicente

Thursday 9:20 Virtual / Track 2 PM17

Rheology and crystallization of Ethylene/Propylene random copolymer (EPR) solutions in mineral oil at varying ethylene/propylene ratio

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In this work we investigate the rheology and crystallization behavior of solutions of Ethylene-Propylene random copolymer (EPR) samples at varying Ethylene/Propylene ratio in mineral oils. A wide range of solution concentration spanning from dilute to semidilute entangled regime was explored. Our results allowed to obtain the c/c* dependence of specific viscosity in a wide range of concentrations of EPR in two different base oils. The reasons for the different thickening power in these oils were elucidated. A precise knowledge of the c/c* dependence of specific viscosity in different base oils is important in lubricants application where polymers are frequently used as Viscosity Index Improvers. Going beyond the well-established results, we also investigated the onset of crystallization in these random copolymer solutions at different temperatures. This phenomenon is also important for lubricant application as the crystallization can severely limit the temperature range of use. The crystallization kinetics and the melting temperature for each tested crystallization temperature was assessed by means of rheological characterization and was correlated to the polymer microstructure. A model derived from Flory's theory of random copolymer crystallization was used to attempt a rationalization of our experimental data in terms of melting temperature vs polymer microstructure.

Thursday 9:40 Virtual / Track 2 PM18

Numerical analysis of the annular backflow in fused deposition modeling

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Fused Deposition Modeling (FDM) is one of the most prominent types of additive manufacturing processes. The polymer filament is pulled into a liquefier where it becomes liquid and is extruded through a convergent capillary die. Annular backflow is one of the most common failure modes. It occurs when the molten polymer can flow back up the annular region between the filament and the liquefier wall, escape the heated area, and cool below its solid/fluid transition temperature. Gilmer et al. [1] proposed a non-dimensional number (Flow Identification Number, or FIN) that predicts a material's propensity to backflow based on a rheological analysis and the system geometry. They concluded that the propensity to backflow is most sensitive to the filament diameter, followed by the degree of shear thinning, in relevant FDM conditions. In spite molten polymers are intrinsically viscoelastic materials, the FIN number was defined based on the power-law model.

It is well known that the fluid-flow of a viscoelastic material throughout a contraction-expansion microchannel exhibit upstream vortices beyond a critical Weissenberg number [2]. In this numerical study, we separately analyze the effect of the elasticity and shear thinning on the formation of upstream vortices during the extrusion flow process throughout an FDM nozzle. The influence of the upstream vortices in the annular backflow is also analyzed. To do so, four different constitutive equations have been considered, i.e. Newtonian, Carreau-Yasuda (inelastic shear thinning), FENE-CR (Boger-like fluid) and Giesekus (viscoelastic and shear thinning) models. Different conventional printing speeds have been considered. Results show that the elasticity enhanced the upstream vortices while shear-thinning inhibited its formation. The formation of the upstream vortices is related to the enhancement of the annular backflow.

[1] Polymer 2018, 152, 51-61.
[2] Materials 2019, 12, 2839.

Thursday 10:00 Virtual / Track 2 PM19

Effects of crosslinking on the viscoelastic response of industrial dual networks

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We have investigated the viscoelastic properties of a series of industrial Pressure Sensitive Adhesives (PSAs), consisting of an acrylate-based polymer and two crosslinkers, permanent (epoxide) and reversible (metal-chelate), with different composition. A combination of shear rheology and a tube-based model (an appropriately modified version of the Time Marching Algorithm, TMA) has been used to probe and analyze their behavior, in particular the effects of the type and amount of crosslinks on the properties of the networks in linear and non-linear regime. To this end, the dynamics of the dual networks were compared with that of the single component (polymer without crosslinks) and that of single networks (bonded by only physical or only chemical crosslinks), in order to quantify their role in altering the relaxation mechanisms, especially the interplay between disentanglement and bond association/dissociation processes. We have examined the influence of TMA model's parameters, such as the lifetime of stickers, polydispersity, molar mass, and, based on the good comparison with the experimental data, we propose a framework to tune material parameters in order to reach a desired viscoelastic behavior. Finally, considering the mentioned studies, by probing the systems with constant shear stress and oscillatory shear stress, we have investigated the effects of crosslinkers on the nonlinear response of the different networks.

Thursday 11:00 Virtual / Track 2 PM20

Flow-Induced Crystallization of a Multi-Block Copolymer under Large Amplitude Oscillatory Shear: Experiments and Modeling

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Following a previous work investigating the flow-induced crystallization (FIC) of polybutylene-terephtalate / polytetrahydrofuran (PBT/PTHF) multi-block copolymers under steady shear, we propose here to deal with the case of large amplitude oscillatory shear (LAOS). For this purpose, we focus on a single copolymer (M_w= 50 kg mol^{-1}) made, in average, of a sequence of nine soft- and eight hard-segments. We show unambiguously that LAOS accelerates the polymer crystallization when increasing (i) the frequency from 0.5 up to 50 rad s^{-1} (at constant strain amplitude of 100 %), or (ii) the strain amplitude from 10 to 300 % (at constant frequency of 2.5 rad s^{-1}). We carefully analyze the stress response through Fourier-Transform decomposition that emphasizes the rich rheological behavior of our material during its liquid-to-solid phase transition. With the help of X-ray scattering experiments (ex-situ SAXS and WAXS), we then propose a global scenario rationalizing the whole set of rheological observations based on the copolymer structure. In parallel, we propose to use a recent model that we developed to simulate the stress response in the case of steady shear promoted FIC and adapt it to the case of LAOS. Remarkably, our model which is based on modified Doi-Edwards equations only, provides good qualitative agreement with the data when varying the strain amplitude or the frequency. Furthermore, it is found to predict quantitatively the gelation time of the system.

Thursday 11:20 Virtual / Track 2 PM21

Wall slippage and the rheological properties of highly filled polymer biocomposites: experiments versus numerical simulations

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Biocomposites are a critical ingredient in the context of overarching societal efforts to increase the use of renewable materials. In particular, the use of biocomposites based on wood fibers as sustainable materials can lead to an impactful reduction in the consumption of plastic materials and subsequently, much less carbon footprint. A current drive for polymer biocomposites is to maximize the use of renewable content in mass production systems. A major challenge therein is to understand the flow field - polymeric matrix/filler, filler-filler interactions, including boundary conditions, in order to design custom processing solutions that enable the manufacturing of parts with desirable performance. In this work, the rheology and processing of commercial highly filled wood fibers-based biocomposites (DuraSense®, StoraEnso) are analyzed from experimental and numerical points of view. The wood fiber biocomposites investigated are based on polypropylene and contain up to 40% wood fiber reinforcement. Their rheological properties are explored using rotational rheometry in simple shear and inline measurements in single screw extrusion. In the extrusion process, pressure buildup in the extruder as well as pressure discharge approximately midway through two different dies (Slit and Film die) have been recorded as input and validation of the numerical results. Further, the experimental findings are compared with numerical simulations. Finite element method simulations are performed using generalized Newtonian and viscoelastic constitutive models, both in the absence and coupled with extensions of the dilute suspension theory for concentrated suspensions (Folgar-Tucker). The study represents a first step towards the implementation of relevant material rheological functions into adequate numerical models for the modeling and optimization of highly filled polymer biocomposites processing flows.

Thursday 11:40 Virtual / Track 2 PM22

Reptation of linear active polymers in melts and concentrated solutions

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The tube or reptation theory is the most successful framework to describe the dynamical response of linear entangled polymers. In this work, we expand the original theory to add the effect of an active force (drift) that acts along the tube, pointing to one of its ends, of a flexible linear chain moving through a mesh of fixed obstacles. We hypothesize that this constant force could be obtained by utilizing active proteins located at the crosslinks of the mesh . By means of analytical calculations, we report that the presence of the constant drift velocity modifies dramatically the dynamics of flexible linear entangled polymers. The magnitude of the drift is restrained to preserve the isotropy of the reptation theory but is sufficiently large to significantly affect the dynamics at long times. The results show an enhancement in the transport properties: the viscosity depends linearly on the molecular weight and the diffusion coefficient of the center of mass depends only on the value of the drift. Moreover, a superdiffusive regime emerges in the mean squared displacement of the center of mass at intermediate distances, whereas the segmental dynamics remain subdiffusive at all times. The results have been obtained by means of analytical calculations and verified by Brownian dynamics simulations. Our results suggest that an active drift could be used to enhance the transport of biomacromolecules through gels or crowded biological media.

Symposium IR

Interfacial rheology, emulsions and foams

Organizers: Anniina Salonen and Nikolai Denkov

Thursday 9:20 Virtual / Track 3 IR17

Phase separation of a confined ionic-liquid – water mixture in a temperature gradient

Marc D. Pascual[1], Alexandre Vilquin[1], and Marie-Caroline Jullien[2]
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Ionic liquids have remarkable properties and are commonly harnessed for green chemistry, lubrication and energy applications. In this paper, we study a thermoresponsive Water - Ionic Liquid (IL) binary mixture which has the property of phase separating above a critical temperature (LCST system). Thermoresponsive Water - IL mixtures have been proposed for various applications such as selective synthesis and extraction of chemical products or desalination. We are interested in the separation process of both phases (in order to recover the phase of interest). For this purpose, we generate a temperature gradient in a microfluidic cavity where the confinement strengthens wetting effects and enhances the demixing. Upon separation an emulsion forms in the cavity and thee two phases rapidly segregate under the effect of the temperature gradient. The temperature dependence of the mixture composition and interfacial tension induce Marangoni strains at interfaces, which are responsible for 3D flows in the cavity. Thermocapillary forces impose the droplets direction of migration while the drainage of wetting films gives rise to shear flows oriented toward the warmer side. Altogether those mechanisms lead to the accumulation of the wetting phase near the heating source. We believe this work will find applications in the recycling of ionic liquids.

Thursday 9:40 Virtual / Track 3 IR18

Breakup of fluid filaments: experiments and numerical simulations

Diana Broboana, István Magos, and Corneliu Balan
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The paper is concerned with the experimental investigations and numerical modeling of the viscous and viscoplastic droplets and filaments breakup in air and in an immersed Newtonian viscous oil. The viscoplastic samples are cosmetic creams, yield stress fluids modeled with the Carreau and Herschel-Bulkley relations. The parameter followed in our investigations is the evolution of the filament neck, and the corresponding thinning velocity, in the vicinity of the droplet/jet breakup. Two flow regimes are observed: (i) an exponential increasing of the neck thinning velocity, followed by (ii) the pinch-off region, where velocity is decreasing or oscillates around a constant value. These observations are correlated with the samples elasticity measured using oscillatory shear and the breakup filaments in CaBER rheometer. The results of this experimental study have potential in developing novel techniques and more precise procedures in determining the interfacial rheology of complex fluid in dominated elongational flows.

Thursday 10:00 Virtual / Track 3 IR19

Study on the formation and thermorheological properties of a novel anhydrous emulsion

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Anhydrous emulsions have been rarely studied and with relatively few publications available, despite having many real and potential applications. Most of their studies focused on the preparation of cosmetic formulations, lubricants, drug delivery systems, etc. Such emulsions also replace conventional ones in applications where the presence of water is undesirable or where higher temperatures need to be reached. Here, stable anhydrous emulsions of polyethylene glycol (PEG4000), with a melting temperature of 58-61ºC, and silicone oil have been successfully obtained. In general, the preparation of this kind of emulsion is not an easy task, due to the phase change during processing and performance and, in addition, due to the difficulty of finding surfactants capable of stabilizing this system, since most of them are destined to water-oil emulsions. However, anhydrous emulsions were successfully prepared with silicone surfactant composed of diblock-copolymers along with bulky silicone chains. In addition, it was possible to obtain largely stable systems over a wide temperature range and for a long period after post-treatment of the emulsion under certain conditions. The objective of the present work was not only to obtain an emulsifiable and stable oil-in-oil system, but also to provide information of how the composition (amount of surfactant and disperse/continuous phase ratio) and the post-processing conditions (processing time and temperature) of the emulsions influence on their final properties. For this purpose, the optical morphology, thermophysical properties and the rheological behaviour of the emulsions were measured and analysed. The obtained results point out especially that operational parameters, such as time and mixing temperature, remarkably affect both rheological properties and stability of the final emulsion. Moreover, some unexpected effects were found related to the miscibility of the silicone surfactant with the disperse phase that yields a modification of the crystallinity.

Thursday 11:00 Virtual / Track 3 IR20

Coalescence in concentrated emulsions: theoretical predictions of bottle test behaviour

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Coalescence is an important problem in emulsions and foams. Classical bottle test experiments are often used to study emulsion stability. Bottle tests consist just in stirring at a given shear rate an oil/water mixture with surfactant, and in measuring after the kinetics of oil-water separation, originating both from sedimentation and coalescence. Several series of experiments have been carefully performed and monitored using on a model system (mixture of brine and dodecane with high amount of surfactant Span 80- w/o emulsion) in order to model its kinetics. We observe two regimes for emulsion separation. The first regime is induced by the sedimentation and fast coalescence of the water droplets, and the second regime where a very dense and stable emulsion is obtained because of slower coalescence at surfactant saturation. At the beginning of this second regime, we show that the thickness of the emulsion zone results from the partition of surfactant between bulk and interfaces. Assuming that the rate of slow coalescence rate depends only on the contact area of the thin film between neighboring two contacted droplets, we quantitatively model the separation kinetics of the dense emulsion zone with only one fitting parameter which is the coalescence frequency per unit area. The predicted value of this coalescence frequency is in good agreement with litterature. Our result shows that a simple measurement of bottle tests could give a very relevant information about physico-chemical quantity of the system of emulsions.

Thursday 11:20 Virtual / Track 3 IR21

Effects of surface viscoelasticity and drop-drop attraction on emulsion rheology

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The rheological properties of emulsions are usually explained by two types of factors - drop capillary pressure (governed by the interfacial tension and drop size) and drop volume fraction [1-3]. However, the interfacial viscoelasticity and drop-drop attraction are two other independent factors which could also affect strongly the emulsion rheological properties. Therefore, we have selected specific saponin emulsifiers which provide highly viscoelastic interfaces and can be used to quantify precisely the effect of interfacial elasticity on the rheological properties of bulk emulsions. Saponins are natural surfactants which are well proliferated in nature and are currently of significant interest for application in food, cosmetic and pharma applications. The obtained results for emulsion rheological properties [4,5] are compared to reference systems with low interfacial viscoelasticity and without attraction between the drops [1-3]. This comparison showed that both the increased interfacial elasticity and the attraction between the drops increase the bulk elasticity of the emulsions up to several times. The most important results, however, is that the combined effect of these two factors is synergistic and the viscoelasticity of the respective emulsion could increase by up to two orders of magnitude, when compared to the reference systems. This synergistic effect could be very useful in various applications, as it increases dramatically the overall stability of the respective emulsions.

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[5] S. Tsibranska et al., *Food Chem.* 316 (2020) 126365.

Thursday 11:40 Virtual / Track 3 IR22

Integrated analysis of the levelling flow of bare circular freestanding liquid microfilms

Massimiliano M. Villone[1], Vincenzo Ferraro[1], Volodymyr Tkachenko[2], Lisa Miccio[2], Lorenzo Lombardi[1], Daniele Tammaro[1], Ernesto Di Maio[1], Gaetano D'Avino[1], and Pier Luca Maffettone[1]
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Freestanding liquid films play an important role in several scientific and technological fields, e.g., biology, materials science, and chemical engineering. In this work, we employ a novel experimental apparatus allowing to produce necked bare circular freestanding liquid microfilms made of highly viscous liquids and then follow their capillarity-driven levelling by means of advanced optical techniques, i.e., digital holography and color interferometry. Experiments on the evolution of the shape and thickness of films made of Newtonian liquids are carried out. The experimental results are effectively captured by a simple model based on the lubrication theory and by finite-element direct numerical simulations, which show that the levelling of the film induces a biaxial extensional flow at its center that, in turn, can be modulated by controlling the geometry of the system. Our computational analysis is, then, extended to viscoelastic liquid films in order to understand the effects of deformation history and fluid rheology on the levelling dynamics.

Symposium MS

Modelling and simulations

Organizers: Natalie Germann and Daniel Read

Thursday 9:20 Virtual / Track 4 MS17

Reinforced elastomers for dynamic applications: from non-linearities to Physics understanding

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Filled elastomers are materials that have been studied extensively by both academics and industrials, and that are now used in a wide variety of applications such as tires or anti-vibratory systems. However, there is still some debates about the Physics involved in the behaviour of the materials under various conditions. One of the remaining question is the dependence of viscoelastic modulus upon the deformation amplitude, known as Payne effect.

A lot of work have been done on this subject in the past years, and most of the community converged on the model of glassy bridges [1]: the mechanical properties of filled elastomers are due to the behaviour of polymer between filler nanoparticles, which acquire a higher Tg than in the bulk (becoming therefore glassy).

In order to understand the behaviour of this material, we analyzed it with the tools that have been developed for the understanding of classical Payne effect: Large Amplitude Oscillatory Shear rheology tests [2], viscoelastic modelling of glassy bridges [1] and plasticization dynamic [3]. We specially focused on the respective role of strain-softening behaviour of one bridge, versus strain hardening. This led to a new understanding of these non-linearity and show how the limited extensibility can be seen in the Payne effect precise analysis.

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Thursday 9:40 Virtual / Track 4 MS18

Constitutive modeling of magnetoactive elastomer

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Magnetoactive elastomers (MAEs) are smart materials whose mechanical properties can be controlled by the application of an external magnetic field. They can be utilized in various engineering applications such as adaptive engine mounts, vibration absorbers, soft actuators, etc. MAEs, which typically consist of micron-sized magnetically soft particles incorporated in a non-magnetic elastomer matrix, yield a coupled magneto-mechanical response at the macroscopic scale when they are subjected to mechanical loadings in the presence of an external magnetic field. Due to the magnetic field, the induced magnetic interactions and the corresponding particle rearrangements vary the mechanical properties significantly depending on the initial particle distribution. This results in a change in the macroscopic shape of the MAE. In our earlier work [1], we studied theoretically the magneto-induced deformation, shape effect, and uniaxial loadings applied to isotropic spheroidal samples along and transverse to the field direction. In this study, we investigate the magneto-mechanical response of the MAE subjected to shear deformation. The MAE yields distinct magneto-mechanical response along and transverse to the field direction, as was already found for uniaxial loadings. The modeling results firmly confirm the transversely isotropic behavior of the MAEs with a random distribution of particles. For such MAEs we propose a transversely isotropic material model as a function of the applied magnetic field and the initial shape of an MAE sample, playing a significant role in the magneto-mechanical response. We thank DFG-Research Training Group 2430 for financial support.

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Thursday 10:00 Virtual / Track 4 MS19

Dynamics and rheology of polymer melts and polymer nanocomposites via simulations across multiple scales

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The study of polymer melts and polymer nanocomposites via molecular simulations is a very challenging field due to the broad spectrum of involved spatiotemporal scales. Here we present a hierarchical multi-scale methodology for predicting the dynamical properties of such systems, that involves detailed atomistic and coarse-grained dynamic simulations. The coarse-grained (CG) models are derived through a "bottom-up" strategy using information from the detailed atomistic scale for the given chemistry. The systematic linking of the atomistic and the chemistry-specific CG models allows the study of a broad range of molecular weights from the oligomers up to entangled systems for specific polymers, without any adjustable parameter [1,2].

As an example we apply the entire methodology to (a) cisPB polymer melts, and (b) cisPB/silica nanocomposites. For both systems we provide a detailed study of their dynamical and rheological properties. We report predictions about the self-diffusion coefficient of polymer chains, the relaxation modulus and the zero shear-rate viscosity for polymer chains probing the transition regime from oligomeric to Rouse-like up to the well-entangled. For the nanocomposites we also examine the dynamical behavior of polymer chains at the polymer/silica interphase by probing directly the segmental and terminal dynamics of the bound layer. The simulation results are compared against experimental data and theoretical predictions.

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Thursday 11:00 Virtual / Track 4 MS20

Molecular simulations combined with theoretical modelling for understanding the microscopic dynamics and shear rheology of unentangled polymer nanocomposite melts

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Molecular simulations are combined with theoretical modeling in order to quantitatively describe local structure, microscopic dynamics and the shear rheology of attractive polymer nanocomposite melts, using as a model system a poly(ethylene glycol) (PEG) - silica nanocomposite melt. First, equilibrium molecular dynamics (MD) simulations are performed to provide insight into the structure of the adsorbed layer around silica nanoparticles, and how this affects the dynamics of the adsorbed and the free chains in the melt. The simulations reveal significant differences depending on the type of PEG terminal groups assumed (hydroxyl versus methoxy), which originate from the different ways that polymer chains adsorb on the silica surface in the two cases. Results from the MD simulations are compared with the predictions of the Rouse model as well as with experimental data for the dynamic structure factor [1,2]. In a second step, well-relaxed configurations from the equilibrium MD simulations are used in large-scale nonequilibrium molecular dynamics simulations (NEMD) under steady shear flow to predict the viscometric functions (shear viscosity and first and second normal stress coefficients) of the nanocomposite melt. The NEMD simulations are further used to parametrize a previously developed theoretical model [3] derived in the framework of the Generalized Bracket formalism of nonequilibrium thermodynamics for the rheology of polymer nanocomposite melts.

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Thursday 11:20 Virtual / Track 4 MS21

From microstructure to soft dense suspensions' rheology

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Soft dense suspensions, as microgels for example, cover a large spectrum of materials made of soft particles immersed in a liquid phase. Although the nature of those solid particles can be very different, dense suspensions share some common rheological properties under simple shear. At densities below but close to jamming density, soft suspensions exhibit shear-thinning. Above jamming, they exhibit a yield stress and their rheology follows a Herschel-Bulkley law. For those materials startup flows can exhibit an overshoot in shear stress which origin isn't well understood. In contrary situations where one stops shearing after flowing, it has been observed that the shear stress of the material eventually relaxes to a stationary value below the yield stress, that is smaller when shear stress applied during the preshear is greater. Establishing an evolution equation for the stress tensor as a response to a given time-dependent deformation is of great importance in order to describe the flow of such systems. Most attempts to obtain a constitutive model are phenomenological. They are typically based on symmetries, such as frame indifference, and while usually motivated by a microscopic physical picture, they do not directly relate the parameters they rely on to microscopic (i.e., particle-level) quantities. The goal of our work is to derive a 2D constitutive model directly from the microscopic dynamics using statistical physics tools. We obtain a Ginzburg-Landau-like tensorial evolution equation on the deviatoric part of the stress tensor coupled with a non-linear time evolution equation on the pressure of the system. This structure predicts a Bingham fluid with the emergence of a yield stress above a critical jamming fraction. The model also shows interesting transient dynamics, predicting stress overshoots upon step increase of the applied shear rate as well as the counter-intuitive dependence on applied shear rate of the residual stresses after flow cessation.

Thursday 11:40 Virtual / Track 4 MS22

The influence of contact line pinning on the structure and rheology of capillary suspensions

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Capillary suspensions [1] are a novel kind of soft matter that offer an attractive processing route to adjust the bulk properties of suspensions. They consist of particles and two immiscible liquid phases where the particles are connected via liquid bridges and form a sample-spanning network. Previous in-vitro experiments have shown that different configurations are possible and a basic dependence on the interaction parameters has been established. However, the influence of the bridge wetting, such as pinned and unpinned contact lines, on the overall stability and yielding behaviour of capillary suspensions is unknown.

Here, we investigate this influence with coarse grained MD simulations using the software Espresso [2]. Capillary forces are described by means of conservative force fields based on toroidal liquid bridges [3] where the pinning of contact lines is achieved by rigid body movement. The networks are formed due to the attractive inter-particle potential during random thermal motion.

We conducted pseudorheological experiments where dynamical properties of our networks were acquired using Lees-Edwards boundary conditions [4], where hydrodynamics is included via the DPD approach [5]. Furthermore, structural properties, like the fractal dimension and the clustering coefficient, are recorded during our in-silico strain sweep experiments. We show that sparser structures are formed when the particles' rotational degrees of freedom are limited and that the linear regime is decreased.

These results can be directly applied in industrial processes where the pinning of contact lines can be tuned by the surface roughness of particles.

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Symposium FB

Food and bio-rheology

Organizers: Jan Engmann and Clément de Loubens

Thursday 9:20 Virtual / Track 5 FB17

Gelation kinetics of aqueous gelatin solutions in isothermal conditions via rheological tools

Pietro Renato Avallone[1], Ernesto Raccone[1], Salvatore Costanzo[1], Marco Delmonte[2], Andrea Sarrica[2], Rossana Pasquino[1], and Nino Grizzuti[1]
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Gelatin is a biopolymer composed of proteins, mineral salts and water. It derives from partial hydrolysis of collagen molecules, which are available in animal connective tissue. Gelatin is a versatile material employed in food, pharmaceutical, photographic and biomedical fields, and it can be used as gelling agent, stabilizer, thickener and texturizer. The thermoreversible sol-gel transition of aqueous pig-skin gelatin solutions at different concentrations and temperatures was explored. In particular, the isothermal gelation kinetics was followed via time sweep tests, close to the critical melting temperature. The latter was previously evaluated via dynamic temperature ramp tests, carried out at different heating/cooling rates. The isothermal analysis allows to evaluate the gel time and to determine its dependence on concentration and temperature. The study of the gelation kinetics over a wide range of concentrations allows to link the behaviour in solution to the gelation phenomenon, confirming a different temperature dependence of the sol-gel transition according to the concentration regime. Although some models are available to describe this dependence, they do not simultaneously account for the effect of both parameters (i.e. temperature and concentration). Here, we propose a full empirical model that includes the gel time dependence upon both temperature and concentration, and successfully agrees with our experimental data.

Thursday 9:40 Virtual / Track 5 FB18

On the inverse quenching technique applied to gelatin solutions

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Gelation is the transition of a liquid solution (sol) into a disordered solid (gel) made up by a three-dimensional network of chemical/physical bonds. This process involves a substantial increase of the viscoelastic properties. Gelatin is a biopolymer widely used in food, pharmaceutical and biomedical fields. It is soluble in water and undergoes a thermoreversible gelation, from a liquid at high temperature to a gel at low temperatures. The sol-gel transition in gelatin occurs via the formation of (physical) junctions among chain strands, even possibly involving coil-to-helix evolution. Gelatin gels are known to be non-equilibrium systems, due to the continuous growth and shuffling of the junction zones, over a long-time scale. This makes hard to perform rheological experiments on a distinct microstructure characterized by a definite number of junctions. Inspired by the inverse quenching technique applied to semi-crystalline polymers and used to measure their rheological properties at a given degree of crystallization, we applied an unusual thermal history to an aqueous solution of gelatin in the semi-concentrated regime (6.67%w pig-skin gelatin). The solution, initially kept in the sol-state at 60°C, is rapidly cooled below the gelation temperature, and isothermal gelation starts at 10°C. After soaking at the quenching temperature for a certain time, the sample is rapidly heated to a temperature value in the range 22-30°C, at which the gelation kinetics is monitored. If the inverse quenching temperature and the low temperature condition duration are suitably chosen, the elasticity (and the relative microstructure) remain stable for a relatively long time. We modeled each step of the inverse quenching technique with a simple second-order reaction kinetics scheme, and we were able to connect the value of the gel elasticity with the resulting crosslinks concentration.

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Thursday 11:20 Virtual / Track 5 FB21

Tailoring the viscoelasticity of polymer gels of gluten proteins through solvent quality

Salvatore Costanzo[1], Amélie Banc[2], Ameur Louhichi[2], Marie-Hélène Morel[3], and Laurence Ramos[2]
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The origin of the unique rheological properties of gluten, the water-insoluble protein fraction of wheat grain, is crucial in bread-making processes and questions scientists since many decades. Gluten is a complex mixture of two families of monomeric and polymeric proteins. To better understand the supramolecular structure of gluten and its link to the material properties, we develop and characterize model gluten using a combination of rheology, biochemistry and scattering techniques.

In this framework, we investigate the linear viscoelasticity of gels produced by the dispersion of gluten proteins in water/ethanol mixtures with various compositions, from pure water to 60% v/v ethanol. We show that the complex viscoelasticity of the gels exhibits a time/solvent composition superposition principle, demonstrating the self-similarity of the gels produced in different solvents. All gels can be regarded as near critical gels with characteristic rheological parameters, elastic plateau, and characteristic relaxation time, which are related to one another, as a consequence of self-similarity, and span several orders of magnitude when changing the solvent composition. Thanks to calorimetry and neutron scattering experiments, we evidence a cosolvency effect with better solvation of the complex polymer-like chains of the gluten proteins as the amount of ethanol increases. Overall, the gel viscoelasticity can be accounted for by a unique characteristic length characterizing the cross-link density of the supramolecular network, which is solvent composition-dependent. On a molecular level, these findings could be interpreted as a transition of the supramolecular interactions, mainly H-bonds, from intra- to interchains, which would be facilitated by the disruption of hydrophobic interactions by ethanol molecules.

This work provides new insights for understanding gluten viscoelasticity and more generally for tailoring the gelation process of complex polymer gels.

Thursday 11:40 Virtual / Track 5 FB22

Rheological properties of chitosan-pectin hydrogels for 3D printing

Iratxe Zarandona[1], Carlos Bengoechea[2], Estefania Alvarez[2], Pedro Guerrero[1], Koro de la Caba[1], and Antonio Guerrero[2]
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3D printing is gaining notoriety as a promising method to process complex biomedical devices. In this regard, natural polymers, such as chitosan, show a soft network and, thus, do not self-support their structures. In order to overcome this drawback thickening agents are needed. Therefore, ink's rheological properties play an important role in 3D printing. In this work, chitosan-pectin hydrogels with different compositions were prepared. The rheological properties of the systems were tested to identify the optimal composition for 3D printing. Frequency sweep tests showed that those systems with chitosan and pectin presented a higher elastic modulus than viscous modulus, resulting in a predominantly solid-like behavior. These results were in agreement with tan delta values at 1 Hz, which were lower than 1 for binary systems and higher than 1 for the systems that only contained chitosan or pectin. Furthermore, elastic modulus at 1 Hz showed the highest value for the system composed of 2 % chitosan and 3 % pectin. Regarding critical strain obtained from stress sweeps, the single systems either with 3% pectin or 2% chitosan showed the highest values, 0.70 and 0.40 respectively, while the values for the mixtures ranged between 0.02 and 0.04, as a result of the solid-like behavior of chitosan-pectin systems. Concerning flow curves, the increase of the viscosity of the systems was dependent of the pectin content and the values in the stationary state were 16,799 Pa·s for the system with 2 % chitosan and 2 % pectin and 37,996 Pa·s for the system with 2 % chitosan and 3 % pectin. All systems showed shear thinning behavior with a flow index ranging between 0.72 and 0.81, except those with 3 % pectin, and were fitted to Williamson model. In sum, results indicated that chitosan-pectin hydrogels with suitable rheological properties for 3D printing can be developed, although these hydrogels should be tested in a 3D printer to check the optimal 3D printing parameters.

Symposium ER

Experimental methods and rheometry

Organizers: Christian Clasen and Mariana Rodriguez Hakim

Thursday 9:20 Virtual / Track 6 ER17

Mechanical investigation of ultrathin polymers

Anastasiia Shpiruk[1], Anne Rubin[1], Mathieu Solar[1], Paul Montgomery[2], and Freddy Anstotz[2]
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Current miniaturization trends in manufacturing requires the understanding of the mechanical behavior as the properties of ultrathin glassy polymers (10-100 nm) differ from the bulk. Many studies have stated that this is a consequence of confinement and/or interfacial physics. We have developed a specific setup based on the nanobubble inflation technique [1] to probe the real time evolution of the mechanical properties by 4D interference microscopy (3D + time). Despite nanoscale issues due to mechanical deformations and drifts, the challenge has been overcome with custom made setup, that allows the control of the temperature, pressure and humidity [2]. In this work using the biaxial inflation method we investigate the environmental effects on the mechanical properties of Polystyrene (PS) and Poly(vinyl acetate) (PVAc), the latter being sensitive to humidity. Ultrathin polymer film are placed onto a substrate that has been etched with an array of 5µm holes. After annealing the sample is placed onto the custom made cell. A static pressure is applied and the deformation of polymer film in the form of the bubble is probed over several hours to measure the change in deformation of up to few hundred nm [2]. The first result is related to the influence of humidity. As expected, the creep compliance of the PVAc polymer films, evolves with moisture, contrary to that of PS. The second result for PS is the emergence of a threshold. In certain cases an unusual behaviour occurs in the form of the inflection of the bubble. The geometry of the bubble shape differs from the usual creeping. To investigate the mechanism of the transition phenomena, a modeling based on a perfectly elastic-plastic law using the Marc Mentat environment is currently being developed. The assumption is that yielding occurs locally.This work will give the opportunity to develop new models to analyse the behaviour of PS and PVAc under different environmental conditions.

[1] P.A.O'Connell et al.,DOI:10.1002/polb.21531.
[2] P.Chapuis et al.,DOI:10.1063/1.5000948.

Thursday 9:40 Virtual / Track 6 ER18

Extensional Gravity-Rheometer (EGR) for yield stress fluids

Anatole Geffrault[1], Hela Bessaies-Bey[2], Nicolas Roussel[1], and Philippe Coussot[1]
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In order to measure the extensional rheological properties of yield stress fluids we developed a rheometrical approach based on the analysis of the deformations of a fluid extrudate falling and breaking in successive elongated drops due to gravity. The flow is filmed at a high frame rate to get a detailed view of the filament shape in time. Assuming gradients of longitudinal velocity are negligible the local instantaneous strain rate is deduced from the variations of the extrudate diameter of each cross-section, while the normal stress is found from the weight of material below this point. The elongational flow curve of the material can thus be directly deduced. The analysis of deformations in the non-flowing region also allows to deduce the behavior of the material in its solid regime, i.e. where the deformations tend to saturate, and the extensional yield stress is found from the position of the transition between the two regimes.

We carried out such measurements with two yield stress fluids with very different internal structures: a concentrated direct emulsion, and a clay (kaolin) paste. In each case the extrusion rate and die diameter were varied, and we measured the stress vs strain rate evolution at any position along the filament. For a given material all the normal stress vs extensional rate data obtained under these different flow conditions fall along a single master curve, proving the consistency of the approach. We thus obtain the extensional flow curve of the material. The results are finally discussed with regards to the simple shear flow curve: it appears that the additional viscous component in the stress (beyond the yield stress) is much larger in elongation than in simple shear.

Thursday 10:00 Virtual / Track 6 ER19

Measuring elongational viscosity of LDPE with elongational viscosity fixture (EVF) up to a Hencky strain of e = 6.3

Masood Khabazian Esfahani, Christos K. Georgantopoulos, Naue Ingo, and Manfred Wilhelm
Karlsruher Institut für Technologie, Karlsruhe 76131, Germany

The elongational viscosity of polymer melts, measured by utilizing the extensional viscosity fixture (EVF) or the Sentmanat extensional rheometer (SER), is currently limited to Hencky strains of e = 4. This limitation arises from the fact that after one complete drum rotation the stretching sample on the drums, falls on itself. To overcome the limitation, a technique is developed in which the sample is placed at an angle of e.g. 45° with respect to the horizon, and thus achieving Hencky strains of up to e = 6.3. A mathematical model is described to incorporate the effect of the sample angle on the stress values as a correction to the obtained values from the rheometer. As an additional approach, the transient uniaxial elongational viscosity of the sample is measured by manually lifting the EVF fixture drums upwards during the experiment, which induces a helical wound up of the stretching sample on the drum. By this method, the sample does not touch itself and the test continues until either the material breaks or the recorded sample torque falls below the instrument sensitivity, which is 0.1 µN.m. The presented methods can be exploited in rheometers to extend the range of application in EVF fixtures by more than 50%. By the two proposed methods, samples with less than 2.4 mm thickness can be tested.

Thursday 11:00 Virtual / Track 6 ER20

Spinning elastic beads: a route for simultaneous measurements of the shear modulus and the interfacial energy of soft materials

Alessandro Carbonaro[1], Kennedy-Nexon Chagua-Encarnacion[1], Carole-Ann Charles[1], Ty Phou[1], Christian Ligoure[1], Serge Mora[2], and Domenico Truzzolillo[1]

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The impact of interfacial stresses on the equilibrium shape of elastic materials can be readily quantified by the elastocapillary length l_e defined as the ratio of the interfacial energy per unit area Γ to the shear modulus G of the body under consideration. When l_e is comparable with or larger than other characteristic lengths of the system interfacial stresses must be considered to compute stationary material shapes or to predict the onset of instabilities. For example, for a hydrogel with shear modulus $G = 30$ Pa and interfacial tension $\Gamma = 30$ mN m^{-1}, the elasto-capillary length is $l_e = 1$ mm. Therefore, the equilibrium shapes of millimetric and submillimetric soft elastic particles is necessarily affected by the interfacial contribution to their total energy.

Unfortunately, for most soft materials the intimate coupling between interfacial and bulk energies hampers the detection of effects solely due to interfacial forces. At the same time, the measurement of the shear modulus is troublesome: techniques like indentation tests, standard rheometry or stretching tests involve the presence of solid–solid contact forces, that affect the measurement and give rise to issues like slip and edge fracture. Here [1] we investigate millimetric beads spinning in a background fluid. We first compute theoretically and then measure experimentally their equilibrium shape using millimeter-size polyacrylamide hydrogel particles introduced in a spinning drop tensiometer. Considering the beads as neo-Hookean up to large deformations, we show that their elastic modulus and interfacial energy constant can be simultaneously deduced from their shape. Our results provide further support to the scenario in which interfacial energy and interfacial tension coincide for amorphous polymer gels.

[1] A. Carbonaro et al., *Soft Matter*, 2020, 16, 8412

Thursday 11:20 Virtual / Track 6 ER21

A high frequency flexure compound piezo device, for integration in a standard rotational rheometer

Bram Schroyen, Florence Müller, Pierre Lehéricey, Christian Furrer, and Jan Vermant

Department of Materials, ETH, Zurich, Switzerland

High-frequency shear rheology provides access to fast dynamics in soft materials and hence can give valuable information about their local scale structure and properties, for example to distinguish between smooth, rough or hairy colloidal suspensions [1,2] or in polymer melts [2]. For systems where time-temperature superposition cannot be used, there is a clear need to physically extend the frequency range beyond what is possible with conventional rotational devices. There has been a myriad of approaches of stand-alone devices which vary in their operating window (T, range of accessible moduli... ; see [3] for a recent review). However, for complex microstructured materials, and for thixotropic materials in particular, the ability to perform a pre-shear is of importance. Furthermore, the low-frequency or non-linear flow properties are of interest as well and it is desirable to have these properties at the same time, or at least on the same instrument on a single sample. In the present work we discuss the design and testing of a rotational Piezo Flexure compound Setup (PFS), constructed to both drive the displacement of and detect the resulting sample response from a single plate by means of an impedance measurement. The aim of the setup is to replace the standard bottom plate in a rotational rheometer and, by using solid piezoelectric elements with limited inertia, to extend the accessible frequency range of SAOS measurements into the kHz region.

[1] Schroyen, et al. (2019). Stress contributions in colloidal suspensions: The smooth, the rough, and the hairy. Physical review letters, 22(21), 218001.

[2] Athanasiou, T. et al. (2019). A high-frequency piezoelectric rheometer with validation of the loss angle measuring loop: application to polymer melts and colloidal glasses. Rheologica Acta, 58(9), 619-637.

[3] Schroyen, et al. (2020). Bulk rheometry at high frequencies: a review of experimental approaches. Rheologica Acta, 59, 1-22.

Thursday 11:40 Virtual / Track 6 ER22

HT-Rheo-E for characterization of liquids at high shear rates

Daniele Tammaro, Salvatore Costanzo, Ernesto Di Maio, Gaetano D'Avino, Nino Grizzuti, and Pier Luca Maffettone

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High-Throughput-Experimentation approach to the rheology of polymer melts (HT-Rheo-E) aims at multi-sample parallel characterization. We report an innovative design of a microcapillary rheometer that is able to perform experiments rapidly, using small amount of material (i.e. milligrams) and on a broad range of shear rates (i.e. from 0.1 to 10'000 s^{-1}). Traditional measurement techniques, as capillary rheometry, require at least several grams of sample fluid. The last years have seen an increased interest in the miniaturization of measurement tools. The novel microrheometer consists of cylindrical microcapillaries in which the fluid is moved by a controlled pressure. A camera, placed at the capillary exit, records the fluid flow from which the viscosity is measured. The optimization of the setup allowed reliable viscosity measurements using less than 10mg of fluids, in few minutes. The oral presentation will illustrate the design of the microrheometer and the viscosity measurements on several fluids.

Acknowledgment: This research forms part of the DPI research programme, project #817'.

Symposium CF

Complex flows

Organizers: Rossana Pasquino and Francisco Galindo Rosales

Thursday 9:20 Virtual / Track 7 CF8

The effect of pulsatile blood flow frequency and microvessel diastole on the endothelial glycocalyx dynamics

Antonis Marousis, Vlasis Mitsoulas, Yannis Dimakopoulos, and John Tsamopoulos

Chemical Engineering, Fluid Mechanics and Rheology, University of Patras, Patras, Greece

The endothelial glycocalyx, a network of membrane-bound proteoglycans and glycoproteins, which covers the luminal surface of the endothelial cells, plays a vital role in vascular physiology and pathology. The oscillated nature of the blood flow affects the functions of the endothelial glycocalyx in either normal or irregular conditions. However, the small scale of the glycocalyx and its complex structure makes it difficult to be examined experimentally. In the present study, we attempt to investigate the dynamical behavior of the endothelial glycocalyx by examining a wide range of frequencies of the pulsatile blood flow, which denote different heart rates. Besides, we account for a more realistic illustration of the capillary, in which the microvessel expands and contracts, and therefore the distance between the glycocalyx fibers variates with time. To do this, we perform 3D Fluid-Structure Interaction (FSI) simulations accounting for both blood plasma and endothelial glycocalyx structural dynamics. The blood plasma is treated as a Newtonian fluid, whereas the glycocalyx fiber is represented as hyperelastic solids. In each case, we evaluate the apparent permeability of the layer and present some characteristic quantities of the glycocalyx fiber dynamics, such as drag force and torque. Our simulations indicate that in high frequencies, the deformation of the glycocalyx fibers is smaller, and therefore the value of the apparent permeability increases. Interestingly, this phenomenon is enhanced while we introduce vasodilation and vasoconstriction on the problem. These results provide a deeper understanding of the glycocalyx mechanisms in real biological tasks and may contribute to the treatment of several diseases, which have been associated with it.

Thursday 9:40 Virtual / Track 7 CF9

Simple model analysis of the effect of shear-thinning and yield stress on the flow of slot coating bead for prediction of slot coating operating limits

Myungjae Lee and Jaewook Nam

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Shear-thinning and yield stress are two important rheological properties in industrially relevant coating liquids, such as suspensions and slurries, and the Herschel-Bulkley constitutive equation can represent them reasonably. In this study, we use aqueous Carbopol polymer solutions as a model Herschel-Bulkley fluid to visualize the slot coating flow. The visualization is performed using a custom-made apparatus that mimics all essential features of industrial-grade slot coaters to detect the location and shape of gas/liquid interfaces and contact lines. Additionally, we develop the simple model of Herschel-Bulkley fluid based on the 1-D viscocapillary model. To understand this system, we should know which dimensionless numbers are governing this system. From the rheological/process parameters, we can get four dimensionless numbers. For low-concentration Carbopol solutions, which shows a weak yield stress behavior, the experimental results and simple model data support that dimensionless number values for the onset of slot coating operating limits are reasonably overlapped. This implies that the dimensionless vacuum is dependent on only Rgt (gap-to-thickness ratio). The system is not sensitive to the change of Bingham number and the capillary number. On the other hand, the result of a simple model analysis implies to us that the yield stress effect is more tremendous when the target thickness becomes thin. With thin wet thickness conditions, the pressure drop occurring through the channel is augmented by the effect of yield stress. This results in the upper shift of the coating window.

Thursday 10:00 Virtual / Track 7 CF10

Bursting bubbles in a yield stress fluid

Vatsal Sanjay[1], Detlef Lohse[1], and Mazi Jalaal[2]

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Bubble bursting in a Bingham fluid is studied using direct numerical simulations. The current system presents a plastocapillarity system in which surface tension and yield stress are the main factors. As the cavity collapses, a train of capillary waves is generated. Viscoplasticity controls the fate of these waves and their interaction at the bottom of the cavity. Unlike Newtonian liquids, the free surface converges to a non-flat final equilibrium shape once the driving stresses inside the pool fall below the yield stress. Details of the dynamics, including the flow's energy budgets,

are discussed. Finally, a regime map is presented, categorizing four main characteristic behaviours. The present study has direct applications in a range of industrial operations, where bubbles are present at the surface of yield stress fluids.

Thursday 11:00 Virtual / Track 7 CF11

How Carbopol microstructure in microcapillary flow is related to yield stress

Raffaele Graziano[1], Valentina Preziosi[1], Behzad Mohebbi[2], Jan Claussen[2], Giovanna Tomaiuolo[1], and Stefano Guido[1]
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Carbopol, is one of the most widely used fluids for the understanding of yield stress origin. Carbopol-aqueous suspensions appear as transparent and homogeneous with the naked eye, whereas high yield stress fluids are commonly quite turbid because of microstructure-based multiple light. Indeed, from the chemical point of view, Carbopol is a high-molecular weight homo-polymer of acrylic acid intramolecularly cross-linked by polyethers, so that, its microstructure is due to the presence of cross-linked gelled polymer particles interacting among each other. Once dispersed in water, Carbopol molecules uncoil, a further stronger expansion (particle swell even more than 10 times of their initial diameter) of polymer chains being due to the neutralization with a suitable base. Indeed, Carbopol in water optical transparency can be ascribed to the remarkable swelling of the particles occurring after the neutralization. In this work, we present a systematic analysis of the microstructure of Carbopol-water solutions under static and flow conditions carried out by mean of confocal microscopy. In particular, we looked at the microstructure of the gel in order to understand the origin of the yield stress and how flow confinement impact on the microstructure. It has been observed that the Carbopol swollen particles build on a 3D network whose connectivity causes yield stress. Furthermore, we have seen that the system can be described as two phases at equilibrium since particle concentration does not influence the properties of the solvent phase. These findings are not limited only to Carbopol aqueous solutions but are also relevant for complex systems based on microgels and polyelectrolytes, and could pave the way for further investigations on the discrepancy between microfluidic results and bulk rheology, likely related to the disruption of the micro-gel structure due to the combined effect of shear rate and confined conditions.

Thursday 11:20 Virtual / Track 7 CF12

Quantifying the destructuring of a thixotropic colloidal suspension using falling ball viscometry

Rajkumar Biswas, Debasish Saha, and Ranjini Bandyopadhyay
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The settling dynamics of falling spheres inside a Laponite suspension is studied. Laponite is a colloidal synthetic clay that shows physical aging in aqueous suspensions due to the spontaneous evolution of inter-particle electrostatic interactions. In our experiments, millimeter-sized steel balls are dropped in aqueous Laponite suspensions of different ages (i.e., time elapsed since sample preparation). The motion of the falling balls is captured using a high-speed camera, and the velocities of their centroids are estimated from the images. Interestingly, we observe that balls of larger diameters fail to achieve terminal velocity over the entire duration of the experiment. We propose a mathematical model that accounts for rapid structural changes (expected to be induced by the falling ball) in Laponite suspensions whose aging time scales are much slower than the time of fall of the ball. For a range of ball sizes and Laponite suspension ages, our model correctly predicts the time dependence of the ball velocity. Furthermore, fits to our model allow us to estimate the rates of destructuring of the thixotropic suspensions due to the passage of the falling ball.

Thursday 11:40 Virtual / Track 7 CF13

Modelling the flow through erodible porous media with SPH

Chaojie Mo[1], Richard Johnston[2], Luciano Navarini[3], and Marco Ellero[1]
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The espresso extraction process involves a complex transport inside a morphological-changing porous medium. Small fines detach from large coffee grains altering the distribution of pores size anisotropically. This process significantly affects the flow and the related extraction profile, so it is important to the final taste of the espresso. In this research, we devise an erosion model in the framework of smoothed particle hydrodynamics (SPH), to take account the erosion of coffee grains. The solid grains are modeled using SPH particles connected by harmonic spring. The springs connecting surface particle are eligible to break under the force exerted by surrounding fluid, so the erosion is considered naturally by the detachment of the surface particles. We examine the relationship between the total erosion rate and the model parameters (the flow rate and the erosion probability). An eroding medium is investigated, the effects of model parameters (the flow rate and the Reynolds number) on the evolutions of porosity, tortuosity and the threshold pressure gradient will be shown. Finally, the possibility to target real systems using X-ray microCT data of coffee capsules will be also discussed.

Symposium FI

Flow instabilities

Organizers: Sandra Lerouge and Mahdi Davoodi

Thursday 9:20 Virtual / Track 8 FI17

Studying shear banding in complex fluids and granular materials with magnetic resonance imaging

Daniel Clarke[1], Daniel Holland[2], and Petrik Galvosas[1]
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Shear banding is a phenomenon observed in some complex materials where distinct shear states coexist. The mechanisms leading to the separation into shear bands, although studied for decades, are still the subject of ongoing research. The study of shear banding benefits from detailed experimental methods - such as magnetic resonance imaging (MRI) - that are non-invasive, spatially resolved and three-dimensional. MRI is also sensitive to velocity fluctuations and the averaged bulk density, facilitating the design of novel experiments to identify the relationship between such parameters and the shear banding behaviour seen in complex flows. Here, we apply MRI to measure the local velocity distribution in Taylor-Couette flows of a wormlike micellar solution and a dry granular flow of plant seeds. Despite being comprised of very different materials, both systems exhibit shear banding, although the physical basis for the formation of shear bands is different. In this presentation, we report on recent results, with a focus on granular flow.

Thursday 9:40 Virtual / Track 8 FI18

Shear banding in cohesive granular materials

Sandip Mandal, Maxime Nicolas, and Olivier Pouliquen
IUSTI, Aix Marseille University, CNRS, Marseille, France

Powders or cohesive granular materials are ubiquitous in industries. However, our understanding of the rheology of these materials is limited. Here, we provide a comprehensive analysis of the rheology of a cohesive granular medium sheared in a normal-stress-imposed plane shear cell over a wide range of shear rate, employing discrete element numerical simulations. At high imposed shear rates, the flow is homogeneous, and the rheology is well-described by the existing scaling laws, involving the inertial number and the "effective" cohesion number [1]. However, at low imposed shear rates, the flow is inhomogeneous, exhibiting the coexistence of flowing and non-flowing regions in the material, known as shear banding. We thoroughly analyze the crucial features of this shear-banded flow regime and discuss striking similarities between the shear banding for granular media and other complex fluids. We reveal that the occurrence of shear banding is related to the existence of a non-monotonic intrinsic rheological curve and that increasing adhesion between the grains increases the non-monotonicity and the tendency towards shear localization. A simple theoretical model based on a non-local rheological model [2] coupled with a non-monotonic flow curve is proposed and is shown to successfully reproduce all the key features of the shear banding observed in the numerical simulations.

[1] S. Mandal, M. Nicolas, and O. Pouliquen, Proc. Natl. Acad. Sci. 117, 8366 (2020)
[2] M.Bouzid et al, Phys. Rev. Lett. 111, 238301 (2013)

Thursday 10:00 Virtual / Track 8 FI19

Interparticle attraction controls flow heterogeneity in calcite gels

Catherine Barentin[1], Sébastien Manneville[2], Teresa Liberto[3], and Marie Le Merrer[1]
[1]Institut Lumière Matière, Villeurbanne 69622, France; [2]ENS Lyon, Lyon 69007, France; [3]Research Area Building Material and Materials Technology, Vienna University of Technology,Faculty of Civil Engineering, Wien, Austria 1040

We couple rheometry and ultrasonic velocimetry to study the flow behavior of gels made of colloidal calcite particles dispersed in water, while tuning the strength of the interparticle attraction through physico-chemistry. We unveil, for the first time in a colloidal gel, a direct connection between attractive interactions and the occurrence of permanent shear bands, as well as large fluctuations in stress and in velocity profiles.

Symposium MS

Modelling and simulations

Organizers: Natalie Germann and Daniel Read

Thursday 11:00 Virtual / Track 8 MS29

Coating die manifold design for viscoplastic materials

Heechan Jung and Jaewook Nam
Department of Chemical and Biological Engineering, Seoul National University, Seoul, Republic of Korea

Many materials such as slurries, pastes, or concentrated suspensions of solid particles in Newtonian liquids often exhibit yield behavior: they can only flow above a certain level of stress. This characteristic can be a problem in a continuous manufacturing process because the material continues to accumulate in the unyielded region and finally damages the products' final quality. In the case of the slot coating process, the flow rates uniformity in the width direction must be made with a high allowance level at the exit of the structure while preventing the solution from accumulating inside the structure called the die manifold. To achieve this objective, we focused on the die manifold flows and the die manifold design.

In this study, we used the Electrical Network Method (ENM) with an optimization scheme to find a minimum of flow rates deviations with a constraint of minimum critical shear rate regions. The ideal Bingham fluid was modeled by the Papanastasiou's viscosity function. The results will be validated through numerical computation based on finite element methods.

Thursday 11:20 Virtual / Track 8 MS30

Finite Element Modeling of the effect of non-Newtonian behavior on contact formation in an external gear pump

Vincent G. de Bie, Martien A. Hulsen, and Patrick D. Anderson
Mechanical Engineering, Polymer Technology, Eindhoven, University of Technology, Eindhoven, Noord-Brabant 5600 MB, The Netherlands

The transport of highly viscous fluids, such as polymer melts, is often performed by external gear pumps. The viscosity of many polymer melts is known to be affected by deformation rate, temperature, and/or pressure. In previous work of the authors [1], the performance of the external gear pump is numerically studied for viscous fluids with different amounts of shear-thinning behavior. In the two-dimensional finite element simulations, the rotation of both gears is imposed. This choice was made due to the complexity of modeling a moving contact point using the finite element method. In this work, the rotation of one gear is imposed, whereas the other gear is freely rotating. The formation of contact in the external gear pump is then studied up to micrometer scale in order to see if a lubrication layer persists for certain processing conditions or material properties. The persistence of a lubrication layer between the gears would result in less wear on the gears of the external gear pump. Processing and material parameters such as rotation speed, pressure difference over the pump and viscosity are studied for a Newtonian fluid. Furthermore, the effect of introducing non-Newtonian behavior, i.e. shear-thinning behavior, temperature and/or pressure dependent viscosity or viscoelasticity, is investigated. When no contact is formed, finite element simulations of multiple rotations of the gears are possible.

[1] V.G. de Bie, M.A. Hulsen, and P.D. Anderson. Finite element modeling of a viscous fluid flowing through an external gear pump. Macromolecular Theory and Simulations, 2020.

Thursday 11:40 Virtual / Track 8 MS31

Influence of rheological parameters on fiber spinning process

Mohammadali Masoudian, Nima Sharifi-Mood, Jean-Marie Marchal, and Petr Kodl
Siemens Industry Software GmbH, Köln 50823, Germany

The fiber-spinning process is an important industrial application to manufacture polymeric fibers. High-speed melt spinning is associated with a neck-like deformation along the fiber and the development of high viscoelastic stresses. Key features to be captured in any model simulation are: radius reduction under high-speed conditions, velocity, viscoelastic stresses, and influence of melt rheology on process conditions. Numerical simulations of non-Newtonian fluids are challenging due to the non-linear form of their constitutive equations and the highly coupled nature of equations associate with stress and velocity fields. In melt spinning process, the constitutive equation must be able to describe adequately the rheological behavior of the polymer in elongational flow. Hence in this work extended Pom-Pom model was utilized to model the rheology of the melt. The parameters associated with this viscoelastic constitutive model was determined based on experimental rheometry data by the means of material calibration solver. An Arbitrary Lagrangian-Eulerian (ALE) method was used to track the free surface of fiber. All steps in setting up these simulations were performed with Simcenter STAR-CCM+.

Symposium MP

Multiphase and other complex fluids

Organizers: Mario Minale and Dganit Danino

Thursday 9:20 Virtual / Track 9 MP17

On the start-up behavior of micellar solutions

Manuela Tonti, Salvatore Costanzo, Giovanni Ianniruberto, Nino Grizzuti, and Rossana Pasquino
DICMaPI, Università degli Studi di Napoli Federico II, Napoli, Italy

Surfactant solutions are used in many applications, as emulsifiers, cosmetics, lubricants, and household products. These molecules assemble in water into supramolecular aggregates, referred to as micelles. The micellar morphology can be tuned by changing some parameters in the system (i.e. salinity, pH, and temperature). The most efficient way to induce morphological and/or structural changes is adding complex salts. The latter can penetrate the micellar core, affecting the effective size of the surfactant molecules, thus inducing a morphological transition from spherical micelles into elongated ones, linear or branched, entangled or unentangled. We report shear startup data on solutions of entangled linear and branched wormlike micelles, differing in concentration and type of two binding aromatic sodium salts. The surfactant molecule is Cetylpiridinium Chloride, at fixed concentration (100mM). Sodium Salycilate and Diclofenac Sodium are used as binding salts, at different concentrations (40-70mM). We proved that the type of salt and its packing effectiveness at the micellar interface are crucial for the dynamics of the wormlike micelles. More specifically, we found that linear wormlike micelles behave similarly to ordinary polymers in fast shear flows, exhibiting pronounced overshoots as well as tiny undershoots in transient shear viscosity, before approaching the steady state. The analogy is emphasized by successfully comparing data with predictions of a constitutive equation, recently adopted for ordinary entangled polymers. Concerning the branched structure, the experimental results in start-up flow strongly depend on the type of salt. In specific cases, the surfactant solutions show flow instabilities and strain hardening. A possible mechanism for the onset of these singularities is proposed.

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Thursday 9:40 Virtual / Track 9 MP18

Experimental and numerical analysis of surfactant dissolution under laminar flow: from microfluidic to pilot-plant scale

Sergio Caserta[1], Ilaria R. Castaldo[2], Benedetta Attaianese[1], Raffaele Rosano[1], Chong Gu[3], Vincenzo Guida[2], and Stefano Guido[1]
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The anionic surfactant Sodium Lauryl Ether Sulphate (SLES) is the main component of many detergent products. Industrial processing of surfactant-based fluids typically includes a dissolution step. Surfactant - water systems typically have complex phase diagram, where at high concentration lyotropic mesophases exhibits complex rheology. As surfactant concentration reduces, molecules rearrange in different phases, each with its own physicochemical and rheological behavior, down to mostly Newtonian micellar solutions in the case of very low concentration. This rheological complexity makes difficult to design dissolution process in flow. This work investigates the dissolution process of SLES pastes in flow in order to find the process controlling parameters that can allow its optimization on the industrial scale. The basic case of surfactant dissolution in a static solvent was recently studied and modelled. Starting from these results, the dissolution process was investigated both experimentally and numerically following a multi-scale approach, starting from a well-controlled microfluidic flow up to pilot plant model scale. In particular, the study was focused on the role of solvent rheology and process flow, investigating the influence of shear stress on the dissolution kinetic. Surfactant dissolution was experimentally measured using flow visualization and image analysis techniques, in the case of microfluidic setup, while solution conductibility and Raman microscopy were used in the case stirred vessels experiments. The flow setup was reproduced numerically by using hybrid models, coupling finite elements methods with analytical models and engineering correlations. Rheological characterization of Water-SLES solution was used to instruct the numerical models. Direct comparison of experimental results with numerical simulations allowed to identify master curve scales able to predict the process outcome on the basis of key parameters, in the of low Reynold number range.

Thursday 10:00 Virtual / Track 9 MP19

Rheological scaling of ionic liquid-based polyelectrolytes in ionic liquid solutions

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Polymerized ionic liquids (PILs) are a special class of polyelectrolytes with ionic liquid (IL) structures on their repeating units. The viscoelastic properties of PILs in IL solutions are strongly influenced by the charge screening by IL ions. However, the effect of IL charge screening on the viscoelasticity of PIL solutions has not been well understood yet, especially at high IL concentrations. In this work, we aim to understand the effect of the counter-anion size and ionic correlations on the rheology of PIL in IL solutions in the semidilute unentangled (SUF) regime.

Specifically, we conduct detailed rheological characterization of three imidazolium-based PILs (PC4-X) in a mixture of salt-free solvent (DMF) and an IL (Bmim-X) consisting of the same side-chain cation, but possessing different counter-anions (X) in size: X=PFSI; large, X=TFSI; intermediate, and X=BF4; small. The specific viscosity (η_{sp}) of PC4-X solutions are measured at various IL concentrations (c_{IL}) in the SUF regime. For the TFSI and PFSI systems, we found that η_{sp} decreased with increasing c_{IL} for c_{IL}<1 M, in good agreement with the behavior of ordinary polyelectrolytes, but η_{sp} increased for c_{IL}>1 M. We captured the observed trend of η_{sp} versus c_{IL} by proposing and validating a modified scaling law accounting for the modified screening length in concentrated solutions. Our model suggests that extended PIL chains initially shrink at low IL concentrations, but revert to expanded configuration at higher IL concentrations due to strong ionic correlations. On the other hand, we observed that η_{sp} for PC4-BF4 solutions decreased asymptotically with increasing c_{IL}, suggesting a finite chain shrinkage due to the intrinsic chain stiffness of the chain. Our results demonstrate that the charge screening mechanism of PILs in IL solutions is different from that for ordinary polyelectrolyte solutions.

Symposium PM

Polymer melts and composites

Organizers: Maria Teresa Cidade and Juan de Vicente

Thursday 11:00 Virtual / Track 9 PM37

Rheological and morphological features of novel LC-copolyesters based on PET

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Among a large number of modern melt-processed polymers, polyethylene terephthalate (PET) remains one of the most important large-scale polyester. Improving the thermal and mechanical properties of PET-based materials can be achieved through chemical modification. Novel thermotropic liquid crystal (LC) copolymers were synthesized by various methods: 1) melt polycondensation in a mixture of diglycol terephthalate and 4'-acetoxy-4-biphenylcarboxylic acid (ABCA); 2) acidolysis transesterification of PET with ABCA. Rather chaotic distribution of comonomer units has been proven by NMR method. Introduction into PET of 40-80 mol. % ABCA provides the production of copolyesters with increased thermal stability (glass transition point - up to 100 °C) and the ability to form anisotropic melts above 270 °C. In copolymers obtained by transesterification, the formation of the LC phase occurs at a lower content of ABCA in comparison with polycondensation copolyesters. In addition, these copolymers are more thermostable and have increased mechanical characteristics (due to the reduced content of ether bonds in macromolecules). According to XRD and polarization microscopy data, the "frozen" LC phase in solid copolymers coexists with crystalline regions of poly-(4'-hydroxy-4-biphenylcarboxylate), non-melting up to 400 °C. The viscoelastic properties of copolyester melts depend on their morphology. At a low content of ABCA units, copolymers form isotropic melts characterized by a quasi-Newtonian flow and a significant predominance of viscous characteristics over elastic ones. Rising the ABCA content is accompanied by an increase in viscoelastic characteristics of copolymers. With the formation of the LC phase in melts, a transition to a non-Newtonian flow with a yield point occurs, as well as an equalization of storage and loss moduli values. Thus, these novel copolyesters can be useful for obtaining heat-resistant materials with an ordered structure.

This work was supported by the Russian Science Foundation (RSF 21-13-00230).

Thursday 11:20 Virtual / Track 9 PM38

Polymeric networks with enhanced mechanical properties

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The increase of mechanical strength of dry polymeric networks presents a significant technological challenge. In general, the increase of the elastic modulus of a material implies a decrease of its ductility. The development of materials combining, high elastic modulus, increased ductility, and enhanced mechanical strength impacts a broad range of interesting applications in plastics, coatings, biomedical devices/implants and products subjected to repetitive stress that may benefit from a material with self-healing properties. In this contribution we present the synthesis of an amorphous, solid linear PEG network bearing two types of bonds, permanent covalent and iron-catechol weaker (potentially reversible) sacrificial bonds. The introduction of iron-catechol bonds lead to an 800-fold increase of the Young modulus relative to the covalently-linked network and provides the necessary dissipation energy mechanism to achieve the desired high mechanical strength. We aim at an in-depth understanding of the above mentioned extraordinary mechanical properties of this double-bonded single network. To this end, we explore the effects of the linear polymer's (PEG or PPO) molecular weight on the morphological and mechanical properties of the network using rheological, mechanical and thermal measurements. Furthermore, we examine the role of humidity that attracts water molecules which compete with catechol for iron binding, compromising the network's mechanical performance.

Thursday 11:40 Virtual / Track 9 PM39

Synthesis and dynamics of double networks based on metal-ligand crosslinks and imine-aldehyde exchange

Rowanne Lyons[1], Larissa Hammer[2], Renaud Nicolay[2], Evelyne Van Ruymbeke[1], and Charles-André Fustin[1]
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Polymer networks are created by cross-linked polymer chains. These links can be either covalent (permanent) or non-covalent (reversible) with consequent effects on the material properties. Both types of networks have advantages and disadvantages: chemical networks resist flow and creep but are difficult to process and recycle, while physical networks are reversible but susceptible to structural changes in the long term. To overcome these limitations, double networks are made of two interpenetrating polymer networks which can be either both covalent, non-covalent or a mix of covalent and non-covalent networks. The combination of a sacrificial first network with a stable and sparsely crosslinked second network offers a balance between extensibility and toughness [1].

In this project, we aim at developing double network elastomers based on metal-ligand supramolecular interactions and reversible covalent bonds [2]. The first network is highly crosslinked by metal-ligand bonds, while the second network is sparsely crosslinked by reversible covalent bonds of the imine type. The dynamics of the metal-ligand complexes can be modulated in a broad range according to the type of metal ions used, while the imine-aldehyde exchange reaction is slower and is only activated at high temperatures.

The networks are studied separately and together using linear rheology in the melt state to understand the effect of the two different dynamics on the structure and properties of the double networks, and the effect of experimental parameters such as the nature of the metal ions and their concentration on the association of the sticky polymer chains.

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[2] Zou, W., Dong, J., Luo, Y., Zhao, Q., & Xie, T. (2017). Adv. Mater., 29, 1606100.

Symposium PG

Powder rheology, granular flows and rheology of solids

Organizers: Alexandra Aulova and Stefan Gstöhl

Thursday 9:20 Virtual / Track 10 PG17

Rheological characterization of fresh concrete – Development of an adaptive rheometer and influence of sedimentation prevention measures

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Due to new challenges in the field of building materials, such as the development of high-performance concrete or predictive simulation, the rheological characterization of fresh concrete on a scientific level becomes more important. However, standard construction site methods (e.g. slump- or L-Box test) and even more precise concrete viscometers (e.g. viscomat or BT) only provide researchers with relative values. This only allows for a relative comparison of different concretes, but absolute rheological properties cannot be measured, which is mostly due to the unpredictable shear fields in these apparatuses. Therefore, the scientific characterization of fresh concrete is not satisfactorily possible up to now. This leads to the need for a scientific grade rheological setup to measure absolute rheological properties.

For this purpose, we developed a coaxial rheometer with interchangeable surfaces to prevent wall slip, which allows the surfaces to be adapted to the investigated material. The dimensions of the rheometer are scaled up to enable measurements of suspensions with particles up to 5.5 mm while maintaining a particle size to gap ratio that does not affect the bulk measurement.

Sedimentation effects are a major challenge when measuring suspensions such as fresh concrete. These effects lead to an inhomogeneous distribution of fresh concrete, which results in hardly reproducible measurement values. To face this problem, we have developed a measurement geometry consisting of a helix-geometry implemented in a groove-geometry. The groove-geometry should inhibit wall slip, whereas the helix-geometry should resuspend sedimented particles, resulting in a homogeneous distribution of the suspension in the measuring gap.

The presented rheometer is by far the first rheometer that focuses on the scientific aspect of characterizing the rheological behaviour of fresh concrete. First results with different fluids (Newtonian, shear thinning and suspensions) will be presented.

Thursday 9:40 Virtual / Track 10 PG18

Evaluating the potential benefits of high cohesivity in powder processing

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Powders are often categorised as being free-flowing or cohesive, with a common perception that highly cohesive materials will experience more processing challenges whereas free-flowing powders will perform well. However, simple flow categories do not describe the breadth of behaviour that powders can exhibit, nor identify how this can change depending on the process environment. Furthermore, perspectives vary on how to quantify 'cohesion'. Shear Cell testing, for example, generates a flow function coefficient which categorises powders into discrete groups and primarily assesses their ability to discharge from hoppers and silos, where higher cohesion will typically inhibit flow. However, hopper discharge is often only the first stage of a manufacturing process, with subsequent unit operations applying a range of stress conditions and flow regimes. Under these conditions less cohesive powders may not always deliver the best results. In certain applications, such as spray coating, dosing and dense phase conveying, a degree of inter-particular bonding and friction is necessary for optimal process performance. In order to optimise productivity and achieve a high quality final product, powders must be selected on the basis of their compatibility with a process, rather than specifying materials using simple parameters that may have little relevance to the process. This presentation illustrates how powder rheology can be used to evaluate flow properties under a range of stress and strain conditions, and demonstrates how this data can be applied to better understand and predict performance in a number of unit operations. The case studies presented also demonstrate how cohesion can be a positive attribute.

Thursday 10:00 Virtual / Track 10 PG19

How to tune the rheology of powders?

Aurélien Neveu[1], Geoffroy Lumay[2], and Filip Francqui[1]
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Numerous industrial applications involve the processing of powders. For example, in the pharmaceutical industry, powder flowability is a key parameter to ensure processability of blends, final tablet strength, mass consistency, or low dose uniformity with the requirement to meet strict specifications for the final product. Being able to tune the rheology of these powders should provide interesting new ways to improve and optimize process quality. In the present work, the influence of additives on the rheology of maize and lactose powders is studied. Modifications of the rheological behavior are evaluated by a rotating drum measurement method involving numerical image processing [1]. Packing dynamics is also investigated with an automated tapped density instrument [2]. Finally, the influence of additive particles on the electrostatic properties of the blends is analyzed with a powder tribocharging device [3]. We show that the inclusion of additive particles significantly modifies the powder rheology and can be used to improve the flowability of the powders. The presence of additive particles at the surface of the grains can drastically influence the cohesive interactions between the grains as well as redesigning the forces network in the assembly. This leads to a major decrease in global cohesiveness and thus a significant improvement in flowability. The rheological behavior can also be tuned from a shear-thickening to a shear-thinning, providing interesting ways to improve processability [3].

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[2] Lumay G, Vandewalle N, Physical Rev Letters, 95, 2005.
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Symposium IR

Interfacial rheology, emulsions and foams

Organizers: Anniina Salonen and Nikolai Denkov

Thursday 11:00 Virtual / Track 10 IR29

Rheology of self-healing organogels of vegetable oils and w/o emulsions

Nataša Šijakovic Vujicic, Josipa Suc Sajko, Ivanka Jeric, Petra Radoševic, and Lidija Brkljacic
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The development of oil gelators has received a huge interest due to their application in food, cosmetics and pharmaceutical industry. Supramolecular gels responding to a mechanical stress offer a wide range of applications in fields such as smart materials, switches, drug release and tissue engineering. We have synthesized chiral oxalamide gelators and investigated their gelation properties in different vegetable oils and water. The organogelators of a present invention showed thermoreversible and thixotropic properties in vegetable oil and emulsions with a minimum gelation concentration of 0.025 wt%. The influence of a length of aliphatic chain and chirality of different aminoacids on the gelator structure causes tremendous differences in a gelation efficacy, self-healing, and rheological properties of the gels in different vegetable oils. Oil gels and gelled emulsions subjected to rheological measurements showed moderate to strong gelation ability examined at very low concentrations from 0.5 to 0.05 wt%. Storage modulus (G') values of gels of 0.1 to 0.5 wt% were in the range from 1 to 100 kPa, and flow point values from 10 Pa to 100 Pa. Frequency sweep studies of the gels indicated that the storage modulus (G') and the loss modulus values are mostly independent of the applied frequency within the linear viscoelastic region. 50 % of the original G' values were recovered in less than a minute for most of the investigated gelators. The properties of the gels were analysed by TEM, SEM microscopy, X-ray scattering, DSC calorimetry and oscillatory rheology. The proof of concept of oil supergelators in food, cosmetics and pharma industry will be presented.

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Thursday 11:20 Virtual / Track 10 IR30

Development of zein-based emulsions stabilized by diutan gum or guar gum. Influence of gum concentration

Jenifer Santos[1], Luis A. Trujillo-Cayado[1], Maria del Carmen Alfaro[1], José Muñoz[1], and Maria T. Cidade[2]
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A by-product from the maize industry, zein, is considered a promising biopolymer of the 21st century. However, zein as a sole material is not suitable for technological applications since it is not flexible enough. The possible solution for extend their applications is the formation of zein-polysaccharide complexes. Firstly, a systematic research about the ultrasonication method on the formation of food emulsions stabilised by zein nanoparticles was carried out. The effect of processing parameters on droplet size was analysed by surface response methodology. Subsequently, the formation of guar or diutan-zein complexes and the influence of their concentration on rheological properties of these food emulsions were evaluated. Guar gum is a well-known biopolymer, and diutan gum is a novel thickener that has been used recently to avoid destabilization processes in lemongrass nanoemulsions [1]. The optimized emulsion was the starting point to form zein-diutan gum and zein-guar gum complexes at different concentrations. Rheological properties as well as the microstructure observed by FESEM were analysed. All emulsions studied showed shear-thinning behaviour and fitted fairly well the Cross model, diutan gum-zein emulsions presented higher values of zero-shear viscosity and lower values of flow index than guar gum-zein emulsions. Furthermore, guar gum-zein complexes did not exhibit gel-like properties since G">G'. As a consequence, emulsions containing guar gum seems to undergo a creaming destabilization process with aging time. In contrast, emulsions formulated with diutan gum-zein presented a 3D-network, observed by FESEM (Field Emission Scanning Electron Microscopy) technique, which was also proved by rheological measurements. This work brings to light the importance of the choice of polysaccharide used in food emulsions formulated with zein.

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Symposium NF

Living and self-assembling systems

Organizers: Daphne Weihs and Jan Vermant

Thursday 9:20 Virtual / Track 11 NF3

Mechanical and structural analysis of channel networks in bacterial biofilms

Steffen Geisel[1], Eleonora Secchi[2], and Jan Vermant[1]
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Bacterial biofilms are formed by communities of microorganisms that are encased by a matrix consisting of self-produced, hydrated extracellular polymeric substances. Biofilm formation is observed in a large variety of microorganisms and provides a protected mode of growth. Recent advances show that biofilms are structurally complex, dynamic systems that exhibit different morphologies depending on the environmental conditions [1]. In certain growth conditions, large three-dimensional structures, which can be defined as channels, are found within biofilms. These channels show low resistance to liquid flow and therefore enable transport by advection [2]. Recent works identify the role of interfacial energy and mechanical instabilities as driving forces during biofilm morphogenesis [3], but the exact mechanism of channel formation is still unclear. Our work represents a step towards understanding the physical process of channel formation within a microbial biofilm. We study how the adhesion of the biofilm matrix to the substrate influences the formation of channels inside Pseudomonas aeruginosa biofilms grown under flow in microfluidic devices. We perform confocal laser scanning microscopy to examine the structure of the biofilm during growth as a function of substrate surface energy. Our results show that biomass production and its adhesion to the substrate control a mechanical buckling instability, which triggers the formation of folds and wrinkles. These three-dimensional structures can be identified as hollow channels in which bacterial movement is greatly facilitated and which rapidly increases the effective volume occupied by the biofilm. Combining methods and concepts from biology and material science sheds light on the physical process of channel formation inside bacterial biofilm grown in flow and enables us to predict and control the biofilm morphology.

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[2] Asally et al., PNAS, 109(46):18891-18896, 2012
[3] Yan et al., eLife 2019;8:e43920

Thursday 9:40 Virtual / Track 11 NF4

The role of shear flow on biofilm morphology

Michela Castigliano[1], Federica Recupido[2], Maria Petala[3], Margaritis Kostoglou[2], Thodoris D. Karapantsios[2], Giuseppe Toscano[1], Stefano Guido[1], and Sergio Caserta[1]

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Biofilms are surface-associated microbial systems showing complex and cohesive structures, providing protection from external environment [1]. Biofilm represents a risk in many industrial processes and in biomedical field. Shear flow affects biofilm formation in different phases of its growth processes by affecting cell attachment/detachment, by regulating mass transport within biofilm structures and shaping their structures. A full understanding of the complex and intimate relationship between the flow intensity and biofilm morphology is still needed.

The aim of this work is to investigate the role of the shear stress on biofilm morphology. Two different experimental setups have been used: a rotating annular bioreactor and a rectangular flow cell-apparatus, both able to impose well-controlled flow conditions. Both are able to impose constant shear stresses on the solid surface where biofilm is growing. Biofilm morphology depends on the environmental conditions, including nutrients availability, that can be affected by medium composition and flow induced transport phenomena. Shear flow furthermore imposes a defined stress on the solid surface.

Biofilm were grown under different flow conditions and the sample morphology and physical properties were systematically investigated. In particular, samples were stained with fluorescent dies, and biofilm morphology was visualized by confocal imaging identifying living and dead cells and polysaccharide matrix [2]. Morphological parameters such as sample thickness and surface roughness were quantified by image analysis. Biofilm wetting under imposed body forces (forced wetting) were also investigated by using a novel device named Kerberos [3].

Biofilm properties were interpreted according to the flow conditions imposed during sample growth, with specific focus on the role of viscous stress at the sample surface.

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[2] Recupido, Colloids and Surfaces B, 2020.
[3] Ríos-López, Coll Surfaces A 2019.

Thursday 10:00 Virtual / Track 11 NF5

A microfluidic platform for characterizing the structure and rheology of biofilm streamers

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In many environmental or medical settings, biofilm formation is the most successful strategy for bacterial colonization [1]. In the biofilm lifestyle, bacteria embed themselves in a self-secreted matrix of extracellular polymeric substances (EPS), acting as a shield against mechanical and chemical insults [2]. When ambient flow is present, this viscoelastic scaffold can take a streamlined shape, forming biofilm threads suspended in flow, called streamers [3]. In many situations, the streamer architecture can enhance the harmful effects of biofilms, bridging the spaces between obstacles in the flow path [4]. Despite their importance for biofilm survival, little is known about the material properties of the matrix. In particular, these are really hard to probe with traditional rheological techniques when the biofilm grows into the thread-like streamer shape.

In this work we present a microfluidic platform that allows to reproducibly grow biofilm streamers in controlled chemical and flow conditions and to characterize their structure and mechanical properties in situ. Our device consists of a straight channel with isolated micropillars, where a bacterial suspension is injected at a constant flow rate. The micropillars act as nucleation points for the growth of a pair of biofilm filaments, developing on the midplane of the channel. The microfluidic technology allows to control the chemical and flow conditions and to perform live imaging of the growth process. We are also able to perform stress tests in situ on the streamers by inducing controlled variations of the fluid shear stress exerted on them by the flow. Thanks to this platform, we are able to investigate the role of the different EPS components and the microenvironment in determining biofilm structure and rheology.

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[4] Drescher et al., PNAS 112,11353, 2015

Thursday 11:00 Virtual / Track 11 NF6

Overview on Staphylococcus aureus cultures rheology during growth

Raquel Portela[1], Pedro L. Almeida[2], Rita G. Sobral[1], and Catarina R. Leal[2]

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Staphylococcus aureus is a mesophilic bacterium that is responsible for a wide range of human diseases, namely the highly successful MRSA (Methicillin resistant Staphylococcus aureus) strains. In the last decade, we have addressed the study of the mechanical behavior of S. aureus cultures, during planktonic growth, under a shear flow. We have explored systematically these systems combining biological approaches with rheology and rheo-imaging techniques [1-4]. In our initial approach, bacterial cultures of S. aureus disclosed a complex and rich rheological behavior not usually accessed by biological analyses [1]. We continued to further explore the effect of several factors, intrinsic or extrinsic to the cell, in the growth process of the S. aureus bacterial cultures, such as: imposition of different shear stresses (stationary and oscillatory) [2]; study of a mutant with a cell separation defect [2]; co-culture growth with E. coli [3]; presence of antibiotics [4] and growth temperature. The presence of particular signatures was identified in the viscosity growth curves and their specific modifications could be related with each considered factor - an overview of these results will be presented. With these studies we aim to bring new insights on the cell-cell aggregation phenomena that may occur during bacterial growth, as well as to contribute to understanding the responses of living cell cultures to environmental stimuli and stresses, which may have repercussions on the infection spreading mechanisms as well as on the developing of alternative antimicrobial strategies.

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[4] Portela R. et al., Fluids 5 (2), 76, 2020.

Thursday 11:20 Virtual / Track 11 NF7

Rheological properties of porcine kidney tissue: measurements and fractional viscoelastic model

Aadarsh Mishra and Robin O. Cleveland
Department of Engineering Science, University of Oxford, Oxford, United Kingdom

The motivation for this work is to develop a fractional viscoelastic model which characterises the rheological properties of kidney tissue. These properties were measured using dynamic oscillatory shear tests, performed using a rheometer (Physica MCR, 302) for frequencies from 0.1 Hz to 9.54 Hz with strain amplitudes from 0.01% to 1%. Kidney tissue was prepared from porcine kidneys within 36 hours of slaughter and a 25 mm diameter sample was extracted from the upper pole, middle pole and lower pole of each kidney. The measured response was deemed to be linear for strains up to 1%. The linear data were fit to a number of viscoelastic models and the best fit was for fractional viscoelastic model which consisted of a 'spring-pot' (fractional order generalisation of spring and dashpot) in parallel with a dashpot. The fractional viscoelastic model was then used to predict the response of kidney tissue to a stress relaxation test. A stress relaxation experiment was carried out by applying a 0.1% shear strain to the sample and the stress measured over 10 seconds. The measured stress was within 22% of the predicted response. In conclusion the rheological properties of kidney tissue have been measured and a fractional viscoelastic model has been described which can be employed in computational models for determining the response of kidney tissue to mechanical insult.

Thursday 11:40 Virtual / Track 11 NF8

Design and flow of biomimetic vesicle prototissues

Laura Casas-Ferrer, Gladys Massiera, and Laura Casanellas
Laboratoire Charles Coulomb, University of Montpellier, Montpellier 34000, France

The aim of this study is to design a biomimetic cohesive tissue with tunable mechanical properties, and to elucidate their role on the overall tissue rheology. We focus in this communication on the role of cell-cell adhesion, which has been shown to be crucial in the flow of epithelial tissues. The artificial tissue is obtained by the controlled assembly of giant unilamellar vesicles or red blood cells, which constitute two suitable model systems for cells. Intercellular adhesion is mediated by the inclusion of different types of ligand-receptor complexes, which allows us to control the occurrence (or not) of cell-cell assembly, the strength of the adhesion, as well as the typical size and morphology of the formed aggregates. Aspiration experiments in microfluidic constrictions are performed in order to characterize the flow behavior of the designed biomimetic tissues. Our results show that, depending on the aspect ratio between the aggregate and the constriction size, the tissue adopts different strategies in order to advance through the constriction: aggregate reorientation, plug-like flows, or cell deformation.

Thursday Afternoon

Symposium PL

Plenary Lecture

Weissenberg Lecture

Thursday 13:00 Virtual / Plenary Lecture PL3

Soft materials designer: where rheology meets chemistry and physics

Michel Cloitre
Molecular, Macromolecular Chemistry, and Materials, ESPCI Paris, Paris, France

Soft materials are all around us. They are present in personal and home care products, food, paints and also in advanced formulations used for enhanced oil recovery, solid ink printing and additive manufacturing. To develop soft materials with tailored properties, formulators combine functional polymers, colloids, emulsions, and amphiphilic molecules, resulting in a great variability of composition, microstructure, and interactions. In spite of their apparent diversity, soft materials share in common the capacity to switch from solid-like behavior at rest to liquid-like under mechanical solicitation. A formidable challenge is to design yield stress glasses or gels with tailored rheology in a rational way. We develop a methodology based on two pillars. On one hand, we take advantage of chemistry to fabricate polymer-colloid hybrids such as microgels, capsules, micelles, star polymers, with variable softness and tunable interactions from repulsive to attractive, leading to a wide range of viscoelastic moduli and time scales. On the other hand, we employ concepts from the physics of disordered out-of- equilibrium materials, in particular jamming transition, supercooled glasses, dynamical heterogeneities, and targeted particle scale simulations to bridge the gap between mesoscopic scale properties, local dynamics and macroscopic rheology. A generic framework emerges, which provides guidelines for designing and engineering yield stress materials with desired properties.

Symposium CS

Colloids and suspensions

Organizers: George Petekides and Valeria Garbin

Thursday 14:00 Virtual / Track 1 CS23

Ring polymers are much stronger depletants compared to their linear counterparts

Esmaeel Moghimi, Maria Kaliva, and Dimitris Vlassopoulos
IESL-FORTH and University of Crete, Heraklion 71110, Greece

Monte-Carlo simulations and mean-field density functional theory suggest that the organization of ring polymers close to walls differs from that of their linear counterparts; in particular, their density profile features pronounced oscillations. Consequently, this leads to a much stronger depletion force for rings [1]. Here, we test this theoretical result and provide unambiguous experimental evidence that rings are stronger depletant agents. We choose an intermediate volume fraction (0.44) colloidal gel based on the classic PMMA hard spheres, in which the depletant is either the linear chain or ring of the same molecular weight. We systematically increase the concentration of the depletant from zero (no attraction) to well above the gelation point and measure their linear and nonlinear viscoelastic properties as the tool to probe the phase transition and strength of the resultant gel. Our results indicate that in the presence of rings, gelation takes place at smaller concentrations. Moreover, the gels made of rings as the depletant are much stronger (higher elastic modulus) compared to the linear ones.

[1] Chubak, Iurii, Emanuele Locatelli, and Christos N. Likos. Molecular Physics 116.21-22 (2018): 2911-2926.

Thursday 14:20 Virtual / Track 1 CS24

A constitutive model for thixotropic aggregating suspensions using population balances

Soham Jariwala, Antony N. Beris, and Norman J. Wagner
Chemical & Biomolecular Engineering, University of Delaware, Newark, DE 19716, United States

Aggregating colloidal suspensions exhibit rheology with distinctive features such as thixotropy, viscoelasticity, and yield stress, much of which can be linked to the complex interactions and kinetics of their mesoscale structures. Population balances offer a more structurally informed statistical approach to connect these rheological features to particle size distributions. This approach uses physically meaningful and independently measurable parameters, and has been shown to work for thixotropic systems such as silica particles and human blood, with prediction accuracy comparable to that of structure kinetics approach. Going forward, it is of interest to establish a correspondence between the particle level information and the model predictions of structure and rheological properties.

As a first step in establishing this connection, we extend the population balance-based constitutive model first proposed by Mwasame et al. [1] to predict the mesoscale structure descriptors like aggregate volume fraction, fractal dimensions, and aggregate size distribution. Using carbon black and silica suspensions as model fluids, we validate the rheological predictions of the model with experimental measurements. Rheological data sets of steady-state and unidirectional large amplitude oscillatory shear (UD-LAOS) measurements are used, following a parallel tempering optimization approach to obtain the fitting parameters for the model. This work provides validation for the underlying physics of aggregation and breakage at the cluster level as well as establishes a modeling approach that uses more structurally informed ab initio principles.

[1] AIChE Journal, **63**, 517-531 (2017)

Thursday 14:40 Virtual / Track 1 CS25

Shear-induced memory effect in colloidal silica gels

Wilbert J. Smit, Thibaut Divoux, Thomas Gibaud, and Sébastien Manneville
ENS Lyon, Lyon 69007, France

We study the influence of shear history on the gelation dynamics and rheological properties of a colloidal silica gel. The colloids aggregate and form a space-spanning gel network upon the addition of salt. After imposing various shear histories during gel formation, we follow the viscoelastic properties over time. Initially, we observe that the gelation process is faster for larger shear amplitudes. The speed-up of gel formation is explained by the mechanical movement, which enhances the mobility of colloidal aggregates and their collision probability. Conversely, at longer times, a high strain amplitude causes a decrease in elasticity and a restructuration of the network structure. The viscoelastic spectra reveal that the newly formed network holds a glass-like structure in which clusters of dense colloids can independently flow. Our results show that shear history can be used to deeply alter and to tune the microstructure of colloidal gels.

Thursday 15:40 Virtual / Track 1 CS26

The influence of aluminum concentration on structure-property relationships of aluminosilicate gels

Jennifer N. Mills[1], Norman J. Wagner[1], and Paramita Mondal[2]
[1]Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716, United States; [2]Civil and Environmental Engineering, University of Delaware, Newark, DE 19716, United States

Cement production and use is one of the leading contributors to anthropogenic CO_2 emissions. Alkali-activated aluminosilicate binders present opportunities for significant reduction in CO_2 emissions, as well as in-situ resource utilization for lunar and Martian construction in support of human space exploration. The chemical composition of these binders impacts macroscopic properties such as workability and strength, but further work is required to connect to the 'geopolymer' formation reaction and microstructure development. The rheological development with time and concentration is crucial for applications including traditional construction processes (pumping, pouring, setting) as well as additive manufacturing. A mechanistic and quantitative understanding of the chemical kinetics and dynamics of microstructure formation and associated rheology development in model geopolymer binders will facilitate the universal engineering of construction materials from a variety of aluminosilicate materials.

The current work focuses on structural characterization of dilute aluminosilicate gel hydrates by relating chemical composition to phase behavior. Gel formation kinetics are simulated through the dosing of the aluminum concentration in solution. Small amplitude oscillatory shear (SAOS) experiments characterize the microstructure development to three phases. Polymer physics are used to predict the gel point, with good agreement to experimental results. Complementary neutron scattering data and NMR show the microstructure responsible for this rheological behavior to scale in a similar fashion, with a change in fractal dimension between phases indicating a shift in aggregation kinetics. The evolution of the gel structure with time and the relationship between structure development and flow are also investigated. These model system studies provide insight into the more complex rheological behavior of dense geopolymer cements and specifically the role of reactive aluminum species.

Thursday 16:00 Virtual / Track 1 CS27

Microstructure-property relationships in carbon black by Rheo-SANS & rheo-conductivity

Julie B. Hipp[1], Jeffrey J. Richards[2], and Norman J. Wagner[1]
[1]University of Delaware, Newark, DE 19716, United States; [2]Northwestern University, Evanston, IL 60208, United States

We explore the shear-dependent microstructure, conductivity, and shear rheology of carbon black suspensions, motivated in part by a desire to predict and control complex rheological and electrical properties in formulations. Direct microstructural measurements over a hierarchy of length scales spanning from nanometers to tens of microns are provide insight into the origin of the suspension viscosity and conductivity across a series of dense suspensions consisting of high-structured carbon blacks from two commercial sources suspended in propylene carbonate and light mineral oil. The shear-induced microstructure was measured at a range of applied shear rates using Rheo-VSANS (Very Small Angle Neutron Scattering) and Rheo-USANS (Ultra-Small Angle Neutron Scattering) techniques. The Bingham number demarcates regimes of stable and unstable flow where in the stable, high shear rate regime, these suspensions exhibit reversible thixotropy resulting from self-similar break up and aggregation of carbon black agglomerates. A shear-thinning viscosity is found to arise due to the self-similar break up of micron-sized agglomerates with increasing shear intensity. This self-similarity yields a master curve for the shear-dependent agglomerate size when plotted against the Mason number, which compares the shear force acting to break particle-particle bonds to the cohesive force holding bonds together. It is found that the agglomerate size scales as R~1/Mn. This inclusion of the particle stress contribution extends the relevance of the Mason number to concentrated suspensions such as those relevant to the processing of carbon black suspensions for various applications. The direct measurement of microstructure with rheology explains why scalings using the Mason number alone are unable to unify diverse thixotropic systems. Similarly, the suspension conductivity under shear flow exhibits classes of behavior that point to differences in underlying mechanisms of charge transfer depending on the system chemistry.

Thursday 16:20 Virtual / Track 1 CS28

Scale-up of the ultrasonication process: CNC dispersion in water validated by rheology

Mélanie Girard, François Bertrand, Jason R. Tavares, and Marie-Claude Heuzey
Polytechnique Montreal, Montreal, Quebec, Canada

Nanoparticle agglomeration is a known problem when dealing with suspensions. Indeed, nanoparticles present a high surface-area-to-volume leading to very strong interparticle forces. One of the widely used methods to overcome this problem is ultrasonication. This process implies cavitation in the medium generating energy levels high enough to break up agglomerates. In a previous work (Girard et al., 2020), we have developed a standardized method to use it efficiently with aqueous suspensions of cellulose nanocrystals (CNC). However, this requires working with small volumes, incompatible with applications at industrial scale.

CNC are bio-based nanoparticles with interesting mechanical and optical properties. But their potential is not yet fully exploited. Even if many articles have been published on interesting results using CNC suspensions at lab scale, transposing these properties at higher scales has proven difficult, namely because of agglomeration.

Thus, in this work, an online continuous process is proposed to treat high volumes of CNC suspensions in water. This approach couples the same standardized ultrasonication method developed earlier with a flow cell. The ultrasonication probe is placed off-centered in a 60 mL beaker allowing for efficient processing, and peristaltic pumps are used to carry the undispersed suspension from a larger container, and the treated suspension back to the main vessel. The dispersion state is assessed via online analysis. Viscosity measurements are carried out using pressure sensors along a capillary, allowing for easy and quick validation of the dispersion state, without requiring additional expensive tools or complex analysis. Moreover, to optimize this scale-up set-up, the flow rate parameter is studied to reach the most advantageous residence time in the cavitation zone where agglomerates are disrupted.

Symposium PM

Polymer melts and composites

Organizers: Maria Teresa Cidade and Juan de Vicente

Thursday 14:00 Virtual / Track 2 PM23

Filament extension atomization – A novel process for powder production?

Moritz Neukötter, Steffen Jesinghausen, and Hans-Joachim Schmid
Particle Technology Group, Paderborn University, Paderborn, Germany

Selective laser sintering (SLS) is inhibited in research by the monoculture of polyamide12 (PA12). New areas of application can only be exploited in connection with improvements in material availability to tackle problems like solvent resistance or elasticity. Also, the powder properties generally have to be within a quite narrow margin for an adequate coating procedure. But, current powder manufacturing processes that yield the necessary powder quality for SLS are specifically tailored to only a few individual polymers, whereas processes under research (e.g., Particles from Gas Saturated Solutions (PGSS)) do not provide the necessary output. In filament extension atomization, individual polymer filaments are continuously stretched at large strain rates ($\dot{\epsilon} > 50\ \mathrm{s}^{-1}$) until instabilities form and decay into droplets even for strain hardening fluids. In this process, the droplets form a monodisperse droplets and rigidify to particles with a high roundness. Introductory experiments using semi-dilute and concentrated Polyethylene Oxide - Glycerol - Water polymer solutions establish a relationship between viscoelastic properties of the solutions and the modal drop size. The formation time of the instability could be determined experimentally from optical measurements via high-speed imaging. Based on the experimental results and the theoretical framework of droplet formation, a model could be established to predict the droplet size at the continuous process filament extension atomizer and will be presented in the talk. The model will allow to perform simulations of the filament behavior depending on the polymer structure with adequate models (e.g. extended Pom-Pom and/or Rolie-Double-Poly) in the near future.

Thursday 14:20 Virtual / Track 2 PM24

Controlling the viscoelastic properties of metallo-supramolecular polymers by combining stickers of different lifetime

Yanzhao Li[1], Flanco Zhuge[1], Christina Pyromali[2], Charles-André Fustin[1], Jean-François Gohy[1], Dimitris Vlassopoulos[2], and Evelyne Van Ruymbeke[1]
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The use of metal-ligand coordination within soft materials forms a very promising and useful class of materials with rich and tunable properties ranging from liquid-like to rubber-like behavior. The viscoelastic properties of these materials are mainly dictated by two synergistic processes: the metal-ligand exchange kinetics and the dynamics of the building blocks (entanglements). In this work, we use entangled telechelic stars of poly(n-butyl acrylate) end-capped with 2,2:6,2"-terpyridine at each chain extremity (Star-PnBA-tpy4) and telechelic linear PnBA (Linear-PnBA-tpy2) as well-defined model systems to form Tpy-Metal complexes once transition metal ions are added. The influence of temperature, nature of metal ions as well as ion content on the linear viscoelastic properties of both single and dual metal ion systems is investigated. In particular, it is observed that the viscoelastic properties of samples containing a large excess of metal ions differ from those of the other samples due to the phase separation of metal-ligand complexes from the polymer matrix induced by the difference in polarity between the charged terpyridine-metal ion complexes and PnBA polymer. The obtained results with telechelic Star-PnBA-tpy4 were also validated based on the linear-PnBA-tpy2 results. We model the linear dynamics of these associating systems with the help of our modified tube-based time marching algorithm (TMA) model by accounting for both the association/dissociation dynamics of the complexes and their possible aggregation, in addition to the entanglement dynamics. This allows us to quantify different species formed in the system and to elucidate their specific role in the relaxation dynamics of the resulting associating systems. On this basis, we assess the association probability of the complexes, in order to rationalize the viscoelastic properties of the resulting materials.

Thursday 14:40 Virtual / Track 2 PM25

Tunable rheology of metallo-supramolecular polymeric networks

Christina Pyromali[1], Flanco Zhuge[2], Yanzhao Li[2], Charles-André Fustin[2], Evelyne Van Ruymbeke[2], and Dimitris Vlassopoulos[1]
[1]FORTH, Heraklion, Greece; [2]Bio-and Soft Matter, Institute of Condensed Matter and Nanos, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

We present a systematic experimental study of the linear and nonlinear shear viscoelastic properties of single and double metallo-supramolecular transient polymeric assemblies with the aim to unravel the role of molecular parameters on the rheological response. Model dynamic networks functionalized with terpyridine ligands were formed by adding different metal ions. The dynamics are driven by entanglement/disentanglement processes and ligand exchange mechanism. Steady state viscosities of single lifetime systems collapse onto a universal curve over a wide range of Weissenberg numbers (from 0.005 to 226). Metallo - supramolecular transient polymeric assemblies consisting of two different metal ions (i.e. lifetimes) exhibit a stronger shear thinning behavior compared to single ion counterparts. The transient shear stress signals exhibit a double overshoot which attributed to the coupled response of the two single network components. The experimental observations are rationalized by analysis based on the use of the modified tube-based time marching algorithm (TMA) of the linear dynamics with the ultimate goal to develop design criteria for tunable single and double responsive networks with improved deformability, coherence and overall network stability.

Thursday 15:40 Virtual / Track 2 PM26

Are unentangled polymer melts simpler than entangled ones?

Giovanni Ianniruberto, Hongwei Liu, and Giuseppe Marrucci
DICMaPI, Università degli Studi di Napoli Federico II, Napoli, Italy

Existing nonlinear rheological data of unentangled polymer melts indicate unexpected features including a significant viscosity thinning in both steady shear [1] and steady uniaxial elongational [2] flows, which are incompatible with existing theories based on the Rouse model, even when accounting for the finite extensibility of the chains [2,3]. Molecular dynamics of melts made of unentangled Kremer-Grest chains also reveal the existence of a nonnegligible second normal stress difference in shear flows [4], the ratio to the first normal stress difference being comparable in magnitude with data on entangled polymers. We here present an effort to describe such apparent anomalies by assuming that a sort of bland topological interaction also may exist in unentangled polymers. In the nonlinear response of shear and elongational flows, Kuhn-segment orientation-induced friction reduction is confirmed to be an important ingredient to describe the observed behavior [5].

[1] Santangelo, P. G.; Roland, C. M. Journal of Rheology 2001, 45, 583-594.
[2] Matsumiya, Y.; Watanabe, H.; Masubuchi, Y.; Huang, Q.; Hassager, O. Macromolecules 2018, 51, 9710-9729.
[3] Ianniruberto, G.; Brasiello, A.; Marrucci, G. Macromolecules 2019, 52, 4610-4616.
[4] Xu, X.; Chen, J.; An, L. Journal of Chemical Physics 2014, 140, 174902.
[5] Ianniruberto, G.; Masubuchi, Y.; Marrucci, G. Macromolecules 2020, 53, 13, 5023-5033

Thursday 16:00 Virtual / Track 2 PM27

Nonlinear shear flow of monodisperse and bidisperse linear polymer melts and solutions

Evelyne Van Ruymbeke[1], Hamid Taghipour[1], Christina Pyromali[2], Laurence Hawke[1], and Dimitris Vlassopoulos[2]
[1]Bio-and Soft Matter, Institute of Condensed Matter and Nanos, Université Catholique de Louvain, Louvain-la-Neuve, Belgium; [2]Institute of Electronic Structure & Laser, FORTH, Heraklion 700 13, Greece

We investigate, both theoretically and experimentally, the nonlinear viscoelastic response of entangled linear polymers under shear flow, in order to better understand the molecular origin of their shear thinning properties and their stress overshoot. To this end, we measure and study the dynamics of monodisperse linear polymers as well as of specific sets of entangled linear blends, using the Cone-Partitioned Plate (CPP) geometry [1]. Based on the shear properties of a long linear polystyrene diluted in an oligomer matrix in various concentrations, we study how the shear thinning properties depend on the long chain concentration. Then, by examining the shear properties of this long linear polymer diluted in a linear matrix of different molar masses, we investigate the influence of this last one on the viscoelastic response of the sample. These experimental results help us to better understand the role of the different components in the shear thinning properties of entangled polymers. We then propose a new approach, based on our TMA tube-based model, to describe the steady viscosity of these samples deformed at constant shear rate. This approach is based on the idea of blobs in shear flow [2]. We show that to obtain quantitative agreement with the experimental data, constraint release effect and chain stretching must be correlated.

[1] S. Costanzo, Q. Huang, G. Ianniruberto, G. Marrucci, O. Hassager, D. Vlassopoulos, Macromolecules 2016, 49, 10, 3925-3935.
[2] Y. Rabin and Rubinstein, M., Workshop on Polymers in strong flows, Capri, July 29-31, 2019.

Thursday 16:20 Virtual / Track 2 PM28

Magnetorheological effects in concentrated soft magnetic polymers

Andrey Y. Zubarev
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Magnetic gels and elastomers feature composite materials consisting of a polymer matrix and fine magnetic particles distributed inside it. Belonging to a family of multifunctional field-sensitive materials, these systems attract significant interest due to an extensive set of unique physical properties they exhibit, valuable for many progressive technologies and making it possible to rank them among 'smart' materials. The dependence of their macroscopic rheological properties on external magnetic fields is one of their fascinating features, attractive from the viewpoint of practical applications and challenging for scientific study. Opening the possibility to control their behavior with the help of moderate magnetic fields ranging from 50 to 600 mT, it makes these composites usable as magnetocontrollable active and passive devices such as actuators, shock absorbers, dampers, etc. Thus, employing magnetorheological/magnetoactive elastomers (MREs/MAEs) as the operating element in various devices seems to be a sound design concept. The macroscopic properties of MAE and their dependence on external magnetic field are determined by the disposition of particles in the host polymer, structures formed by them, structural transformations occurring under the influence of the field, and large-scale deformations suffered by the material. Analysis of the literature indicates that despite the fact that investigations dedicated to the magnetorheological (MR) effect are numerous and the overall data collection is huge, the information available does not suffice for making the complete picture. The present work is focused on the search for new compositions with high MR properties, experimental and theoretical study of the relationship between their micro-and mesoscopic structure with the macroscopic MR effects.

Symposium IR

Interfacial rheology, emulsions and foams

Organizers: Anniina Salonen and Nikolai Denkov

Thursday 14:00 Virtual / Track 3 IR23

Elastic overshoot in liquid foam flows through and around a permeable defect.

Lauren Rose[1], Natalia Shmakova[2], Christophe Raufaste[3], Benjamin Dollet[4], and Stéphane Santucci[1]
[1]Laboratoire de Phyique, ENS de Lyon, Univ Lyon, CNRS, Lyon, France; [2]Lavrentyev Institue of Hydrodynamics, Novosibirsk, Russia; [3]Université Côté d'Azur, CNRS, Institut de Physique de Nice, Nice, France; [4]Université Grenoble Alpes, CNRS, LIPhy, Grenoble, France

We present an experimental study of a two-dimensional liquid foam, composed of a confined monolayer of bubbles, forced to flow within an inhomogeneous open fracture, at a constant rate. Our model porous medium consists of a Hele-Shaw cell with a single localised defect that completely fills, reduces or expands locally the cell gap, and therefore, either decreases or increases locally its permeability. The transparent glass panels of the cell allow a direct visualization and tracking of the elementary components of the foams, the bubbles, through the observation of their films and vertices.

Analysing the evolution of the liquid foam properties (and more specifically, the displacement and shape of the bubbles), we compute the average steady-state velocity and bubble deformation fields of the flowing foam. We investigate here the influence of the geometry of the defect (height, size, and shape) on the average steady-state flow (velocity and deformation) of foams of various liquid contents (from very dry foams to very wet ones close to bubbly liquids).

In the frame of the flowing foam, we can observe a recirculation around the defect. The velocity field displays a strong fore-aft asymmetry, with an extended region downstream the defect, where the foam velocity can be significantly larger than the imposed driving one. Furthermore, we show that this velocity field is clearly correlated to the bubble deformation field, with in particular, the amplitude of the velocity overshoot proportional to the maximum deformation of the bubbles.

Our experiments confirm that the elasto-plastic properties of liquid foams, which are notably controlled by their liquid fraction, are at the origin of the fore-aft symmetry breaking of the flow, triggered by the defect, and paves the way towards the development of a theoretical approach, allowing to predict this velocity overshoot as a function of the mechanical properties of the liquid foam (shear modulus and yield stress).

Thursday 14:20 Virtual / Track 3 IR24

Impact of surfactant concentration on the deformation of a soap film assembly

Raphael Poryles, Théo Lenavetier, Adrien Bussonnière, Emmanuel Schaub, and Isabelle Cantat
Institut de Physique de Rennes, Rennes, France

Foam is used in many processes, for instance, in the food industry and for oil extraction. The bulk rheology of foam shows a complex behaviour, and one issue is to connect this global rheology with the rearrangement of the bubbles and the interstitial films at the local scale. To model those local deformations, we construct an assembly of five soap films on an X shaped frame (one central and four lateral). The foaming solution is made of a mixture of two surfactants: SDS and dodecanol. The SDS is soluble and allows us to build the film assembly while the addition of dodecanol which is almost immiscible provides interfacial elasticity to the films. The four lateral films are fixed on individual piezoelectric motors allowing them to be extended and compressed at will. By pulling the two lateral films on one side and pushing the ones on the other side, we observe a displacement of both menisci. By a force balance, we compute the tensions in each individual film. We also observe in the central film the extraction from the menisci of a thicker film. In previous work from our group [1] a model was constructed to connect this thick film extraction and the tension of the different films using the interfacial elasticity. In the current study, we investigate the impact of the different surfactant concentrations on the elasticity of the different films. By tuning the concentrations, we show that the elasticity increases with the dodecanol concentration while it decreases with the SDS one. Knowing the film extensions, we compute the surface concentration of each specie and build a physicochemical model that shows quantitatively an agreement between the tensions measured experimentally and the ones predicted by mass conservation during the compression/extension of the films. Those results for those two specific species confirms that our setup can be used to measure precisely the dynamical interfacial rheology of soap films and such study will be extended for more complex surfactants.

[1] Bussonnière & Cantat, arXiv:2011.13658

Thursday 14:40 Virtual / Track 3 IR25

Stability of marginal pinching in soap films

Corentin Tregouet and Isabelle Cantat
Soft Matter Department, Univ Rennes, Institut de Physique de Rennes, Rennes, France

The stability of soap bubbles and hence of liquid foams is a set by the film thinning, which is known to occur locally: rounds patches of thin films appear at the edges of the film before moving to the top of the film by buoyancy. This phenomenon, the marginal regeneration, has been observed for decades, but its origin hasn't yet been established. It involves the appearance of a localized pinch between the film and the meniscus, which dynamics has been entirely characterized by assuming its invariance in the direction of the meniscus. We identify a limit in which the bulk drainage and the surface rearrangements are decoupled, the film thus evolving in a sliding-puzzle-like dynamic. In this frame, we study theoretically and numerically the stability of this straight marginal pinch, and show that it is unstable to long wavelengths. We predict a critical wavelength of fastest destabilization and a thickness ratio between the thin and thick parts of the film, both in good agreement with experimental observations.

Thursday 15:40 Virtual / Track 3 IR26

Rheological criteria to predict polymer foamablity using ScCO2

Benoit Rainglet[1], Veronique Bounor-Legare[2], Yvan Chalamet[1], and Philippe Cassagnau[2]
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Polymer foams have a major role to reduce the consumption of plastic and to enhance mechanical properties, thermal insulation, etc.... Basically, foaming can help us having the same result or better with less material. Foaming can occur through two ways, chemical, a chemical reaction produce gas like during the formation of PU foam, and physical, which is to use a dissolved physical agent, which go through instability and create bubble while undergo a thermodynamic instability produced by an increase of temperature or a reduction of pressure. The use of CO_2 as a physical blowing is not new, nevertheless the prediction of the foamability of a polymer is not completely achieved. So there is a need for simple criteria depending of the physical property of the polymer which can be easily measure to predict the foaming behavior of polymers. Our work is to use rheological measurements, linear shear and non-linear elongational, to predict the foaming behavior of different Polypropylene formulations having really different rheological behaviors. Based on different PP formulations, we defined two rheological criteria for linear and non-linear rheological behaviors. We showed from some foams examples (cell morphology and foam density) that these criteria are really relevant can be used to optimize the polymers formulations.

Thursday 16:00 Virtual / Track 3 IR27

In situ generation and rheological characterization of dynamically-aging foams using 3D-printed fractal vanes

Igor M. Carraretto[1], Crystal E. Owens[2], Luigi P. Colombo[1], and Gareth H. McKinley[2]
[1]Politecnico di Milano, Milano, Italy; [2]Massachusetts Institute of Technology, Cambridge, MA, United States

Foams are employed in a wide range of different fields, from food processing and cosmetics to advanced metallurgy, and recently they have been adopted into the oil and gas industry as liquid loading reducers. However, an accurate and precise rheological model for the foam is required in order to understand and eventually simulate the complex multiphase flow dynamics that evolves during transport in a pipeline - where liquid, gas and foam are all present concurrently. In order to reproduce the key features of the transient foam generation and flow process and eliminate flow-history artifacts induced by sample loading of the foam in a rheometer, an experimental setup has been developed that allows *in situ* generation and characterization of low liquid-phase volume foams. We use stereolithographic additive manufacturing to print fractal, multi-arm vane tools that eliminate slip at the interface with the tooling and reduce stresses exerted on the foams, as well as to manufacture baffled cups that incorporate a foam-generating mechanism *in situ*. We use these fixtures to measure the evolution in the foam viscoelasticity and the progressive decay in the yield stress and relate these to the evolution of the bubble size distribution over time. We study two aqueous foams: Gillette shaving foam, and a commercial flow assurance product by Chimec S.p.A. utilized in the oil and gas industry. Our results show that after an induction period set by the drainage of the liquid in the bubble cell walls, the mean bubble radius in each foam increases over time as $t^{0.5}$, in accordance with previous measurements. Rheological measurements of the resulting evolution in the yield stress and the entire flow curve show that the aging and coarsening processes in these weak aqueous foams are self-similar and can be described with good accuracy by the well-known Princen & Kiss model, in conjunction with a single age-dependent shift factor whose evolution is controlled by the Sauter mean bubble radius.

Thursday 16:20 Virtual / Track 3 IR28

Thin liquid films: where hydrodynamics, capillarity, surface stresses, and intermolecular forces meet

Emmanouil Chatzigiannakis[1], Nick Jaensson[2], Patrick D. Anderson[2], and Jan Vermant[1]
[1]Department of Materials, ETH, Zurich, Switzerland; [2]Department of Mechanical Engineering, Eindhoven University of Technology, Eindhoven, The Netherlands

Thin liquid film (TLF) dynamics is considered to be the governing factor when it comes to the stability of multiphase materials, such as foams, emulsions and immiscible polymer blends. When two bubbles come into close proximity a TLF is usually formed between them, which gradually drains. The drainage process and, consequently, the stability of TLFs has been found to depend heavily on the surface stresses of the interface. However, the exact ways by which surface stresses due to Marangoni, surface viscosity and surface viscoelasticity act remain unclear. In this study we combine (i) experiments with the dynamic thin film balance technique and (ii) FEM simulations to study how exactly surface stresses affect the drainage. The use of model systems allows us to decouple the effects of disjoining pressure, surface stresses, capillarity and hydrodynamics. New insights on the influence of surface stresses are provided, with a specific focus on how surface rheology can affect film dynamics. Previous, seemingly contradicting, results in literature are also rationalized.

Symposium MS

Modelling and simulations

Organizers: Natalie Germann and Daniel Read

Thursday 14:00 Virtual / Track 4 MS23

Tensorial models for shear jamming and yielding for generic geometries

Giulio G. Giusteri[1] and Ryohei Seto[2]
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The rheology of concentrated suspensions presents us with a formidable challenge as far as continuum modeling is concerned. In spite of our great advances in understanding the microscopic origin of surprising phenomena, like discontinuous shear thickening and jamming, the variety of macroscopic phenomena observed in suspensions remains difficult to capture with a single continuum theory.

Within this work, we address the definition of continuum models that are capable of reproducing shear jamming and fragility [1,2,3]. These are two aspects of the dynamic evolution of the suspension microstructure that are characterized, in their simplest manifestation, by a jammed state, built by applying a constant shear stress, that behaves like a solid under a stress aligned with the building one, but flows again if the stress is reversed.

The framework that we employ [4] turns out to be useful also in describing yielding phenomena, that can occur in suspensions under high stress or due to the presence of attractive interactions among the particles, and provides a simple starting point for more complicated models.

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[3] Seto, R., Singh, A., Chakraborty, B., Denn, M.M., Morris, J.F.: Shear jamming and fragility in dense suspensions. Granular Matter 21, 82 (2019)
[4] Giusteri, G.G., Seto, R.: Shear jamming and fragility of suspensions in a continuum model with elastic constraints (in preparation)

Thursday 14:20 Virtual / Track 4 MS24

Mikto-arm stars interconnected as soft patchy nanoparticles: Atomistic simulation study

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In the world of nanostructured particles, patchy-like structures represent a family of building blocks with multiple spatially distributed segregated regions. Thanks to this feature, patchy nanoparticles have emerged as a novel class of building units to conceptually enable the design of self-assembled macro-objects, that is achieved by the soft and directional interactions that arise between the patchy regions. Recently, we reported [1] that a single-molecule 32-arm star composed of alternately connected poly(ethylene oxide) and polystyrene arms (PS/PEO stars) nanosegregates into a patchy-like particle in an unfavorable environment for both components.

Here, we present an atomistic simulation study of multiple-star systems consisting of PS/PEO mikto-arm stars with a patchy-like morphology. Unlike other examples of patchy-like structures, e.g., multicomponent hairy particles, the mikto-arm stars are penetrable and intramolecularly nanosegregated, thus the patches are fully interconnected when incorporated into a self-assembled structure. By varying the number of stars in the system, we aim to examine systematically the directional segregation of the star-like building blocks.

The individual stars preserve their morphology and shape when they link into a multi-star macromolecular object. We detect and characterize various patterns and types of mutual orientation of the particles. Our results represent the first evidence that the mikto-arm stars can be used as building blocks with the patchy-like morphology in the macromolecular design and reveal possible attachment of these particles in the assembly.

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Thursday 14:40 Virtual / Track 4 MS25

Computer simulations of packed soft colloids with thermal motion

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Soft colloids are micron-scale structured objects such as polymer microgels, that are compressible and deformable. Even at high packing ratios a soft colloid may still be able to undergo cage-breaking due to particle deformation. The link between the detailed elastic properties of soft colloids and the resulting dynamics are presently not well understood. Soft colloids show rich rheological behaviour and we wish to understand the links between the single particle elastic properties and the resulting rheology. We use a recently developed algorithm, Fluctuating Finite Element Analysis, for simulating viscoelastic objects undergoing thermal excitation. While symmetric soft particle potentials have been much studied, our approach captures the detailed shape deformations of the colloidal particles so that the structure and anisotropic deformation of the particles are taken into account. We are able to explore both variations in particle modulus and volume fraction. In the particle mean squared displacement we find evidence of cage-breaking events even where the effective volume fraction exceeds the close packed limit. We examine stress relaxation in the linear regime and are able to decompose the relaxation modulus into structural and intra particle contributions and study the scaling of these with particle modulus and volume fraction. Additionally, we present simulations of steady shear, examining both the stress and the structure via scattering function.

Symposium FB

Food and bio-rheology

Organizers: Jan Engmann and Clément de Loubens

Thursday 14:00 Virtual / Track 5 FB23

The influence of dispersing system on rheology and microstructure of dietary fibre suspensions

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The interest towards dietary fibre is continuously growing owing to both its nutritional (reduction of risks associated with different gastrointestinal or cardiocirculatory disorders) and technological (ability of structuring water building a three dimensional network) effects. The gelling ability of fibre is related to the hydration of particle cell walls and to the formation of particle clusters that grow and build the network. As a consequence, the system used to disperse fibre in water and the adopted concentration can affect in a relevant way the rheological properties of the final suspensions. In this work two different devices, a rotor-stator system and a Microfluidizer, were used to prepare fibre suspension at increasing concentrations to investigate the potential effects of different dispersing methods. Rheological characteristics of obtained samples were studied with small amplitude oscillations; optical microscopy and light scattering were used to investigate the effectiveness of particle dispersion, whereas suspension stability was studied through multiple light scattering measurements. It was observed that, when a high-energy input is used, the rheological characteristics are almost independent of the adopted device whereas particle dispersion is slightly different. A simple rheological model was proposed to relate dynamic moduli and fibre concentration with the aim of proposing a tool useful in designing suspensions having the expected rheological properties.

Thursday 14:20 Virtual / Track 5 FB24

The importance of rheology in the development of rice bran-based bioplastics via injection moulding

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The agro-food industry produces huge amounts of wastes and by-products mainly employed in animal feed, being low added value residues. These by-products account for high levels of proteins and carbohydrates, basic food groups that, properly treated, can be employed for the development of bioplastics through thermo-mechanical methods. By these means, they are transformed into high added value products that also exhibit environmental advantages as they represent an alternative to traditional fossil-based polymers (mostly non-biodegradable). In this research work, rice bran, a by-product from rice processing, is selected due to its high protein and carbohydrate contents. The rice bran is mixed with glycerol and water, acting as plasticizers to obtain homogeneous doughs that can be processed into bioplastics via injection moulding. The mixing temperature is a key parameter that will affect the properties of the doughs and thus, the final specimens. In this way, the main objective of this work is to select the proper processing conditions (mixing temperature) and, to this end, both doughs and final bioplastics are subjected to oscillatory tests. In addition, the final bioplastics are also evaluated through tensile tests, water uptake capacity tests and Scanning Electron Microscopy. The rheological characterization revealed mechanical improvements observed for the highest mixing temperature employed (110 ºC) in the dough without ageing that, at the same time, exhibited poor physical integrity after water immersion. On the other hand, the rheological properties of the aged doughs improve when the temperature raised to 80-90 ºC, especially for the first one, showing lower values for the doughs mixed at 50 and 110 ºC. Although the mechanical properties of the aged system obtained at 80 ºC are slightly lower than those obtained for the non-aged dough formed at 110 ºC, these specimens are considered more appropriate since they exhibited higher physical integrity and, as a consequence, better-operating conditions.

Thursday 14:40 Virtual / Track 5 FB25

Pasting properties of fura extrudates from pearl millet and blends of grain legumes

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Fura is a Nigerian traditional food usually prepared from cereals (pearl millet, sorghum or maize). Fura was produced using the traditional process from 100 % pearl millet flour as a control. Seven extrudates representing single 100% pearl millet and 6 blends of pearl millet flour with three-grain legume flour mixtures (cowpea, soybean, and groundnut) at 20 and 30 % levels were extruded. Fura is a single cereal product, limiting in the essential amino acid lysine. To mitigate this challenge the grain legumes were added to complement the amino acids profile. The gelatinization temperature ranged from 62 - 70.7 ºC for pearl millet: cowpea (80:20) and 100% pearl millet traditional fura. There was general decrease in the gelatinization temperature of fura extrudates when compared with non extruded 100% pearl millet fura, suggesting the decrease because of the previous gelatinization of their starches during extrusion process. Apparent viscosities equally show drops in the values for fura extrudates because of damage done to the starches during extrusion. At 30oC the apparent viscosities of the products ranged between 4.2 - 17.6 Nsm^{-2} for pearl millet: groundnut fura (80:20) and 100% pearl millet non extruded fura. There were no significant differences in the apparent viscosities of extruded fura samples ($P<0.05$) at 30 ºC. The set back value (retrogradation) sowed values between - 60 to 170 Bu for millet: cowpea (80:20) and 100% traditional non extruded fura. The ease of cooking ranged from 12 - 25 minutes for pearl millet: cowpea fura (80:20) and 100% pearl millet non extruded fura; suggesting that the energy consumption during preparation is reduced by extrusion. The Viscosity after cooling from 92 ºC to 52 ºC ranged from 20 to 250 Bu for pearl millet: soybean fura (80:30) and 100% pearl millet non extruded fura respectively. The Viscosity after 15 minutes at 92 ºC ranged from 20 to 90 Bu for pearl millet: cowpea (80:20); pearl millet: cowpea (70:30); pearl millet: soybean (70:30) and 100% pearl millet non extruded fura.

Thursday 15:40 Virtual / Track 5 FB26

LAOS results obtained with commercial chocolates: Application to thixotropic yielding flow

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In this work we have investigated the linear viscoelastic properties, yielding, and shear-thickening behavior of commercial molten chocolates. SAOS measurements reveal that the chocolates display a very narrow linear viscoelastic zone, evidencing the need for focusing on the more extended nonlinear region, where moderate and large deformations are applied. Actually, processing and consumption of chocolates imply large

and rapid deformations and, hence, the response should be dependent on nonlinear characteristics [1]. During Large Amplitude Oscillatory Shear (LAOS) measurements, in strain-controlled experiments, the stress response is not sinusoidal, so another treatment is necessary. Four approaches have been used in this work:
1) Use of the normalized third harmonic (I3/I1), through the zero-strain nonlinear coefficient Q_0 [2],
2) Generation of Lissajous curves and further decomposition of stress into their elastic and viscous components using Chevyshev polynomials of the first kind [3],
3) Stress-strain limit yielding parameters interpreted by means of the geometric average of Lissajous curves following stress bifurcation analysis [4], and
4) Analysis of temporal stress signals in terms of a sequence of physical processes (SPP)[5]. With these approaches a sound rheological analysis of the nonlinear region has been performed establishing a liaison with the chocolate microstructure. The results are interpreted considering the contribution of both, particle size distribution bimodality and fat content, to the thixotropic yielding flow of chocolates.

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[2] Hyun, K. and Wilhelm, M. (2009) Macromolecules, 42, 411-422.
[3] Ewoldt, R., Hosoi, E., & McKinley, G. H. (2008) Journal of Rheology, 52, 1427-1458.
[4] Yang, K., Liu, Z., Wang, J., and Yu, W. (2018) Journal of Rheology, 62, 89-106.
[5] Rogers S.A., Erwin B.M. Vlassopoulos D. and Cloitre M. (2011) Journal of Rheology 55, 435-458.

Thursday 16:00 Virtual / Track 5 FB27

Characterizing plant-based gels with DWS microrheology

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In the last 10 decades of food technology, yogurt ranked first among the entire cultured dairy products in terms of dairy industrial production and research studies[1]. Despite its established health benefits, consumers' interests are increasingly changing towards plant-based dietary products. The development of non-dairy yogurt from various plant sources comes with challenges such as textural inconsistencies. There is a lack of knowledge about the effect of various proteins and thickeners addition on the rheological properties of non-dairy yogurts, stimulating new research efforts. In this context, the DWS technology offers considerable advantages in characterizing formulations. Very small sample quantities, as well as very fast measuring times, allow an increase in the number of screenings by up to 10 times compared to classical mechanical rheometers. As the samples are sealable, the technology also allows the simple and reliable measurement of aging, gelling, and agglomeration processes. We present applications of DWS-microrheology on plant-based gels. In particular, we demonstrate the ability to record very subtle changes in the structural properties. We also show that the rheological properties can be recorded over a huge frequency range at acquisition times of about 3 minutes.

Symposium ER

Experimental methods and rheometry

Organizers: Christian Clasen and Mariana Rodriguez Hakim

Thursday 14:00 Virtual / Track 6 ER23

Rheological setup for in situ real-time crosslinking gelation.

Ioanna N. Besiri, Thomas B. Goudoulas, and Natalie Germann
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In situ rheological research can give significant insights into the time-dependent gelation. For this purpose, we recently proposed a method for *in situ* real-time crosslinking reactions [1]. Our setup consists of a custom-made lower-rheometric plate of two parts made of stainless steel (SS) and a standard upper cone. A volumetric syringe fills the cavity of the SS parts with the ions through the side. An upward flow delivers the ions through four micro-scale holes at the top of the setup via a channel configuration to induce the chemical gelation with the polymer located on the outer surface of the setup. The advantages of the method are the control of both the concentration and volume of the crosslinker and precise measurement the gelation kinetics.
In our study, we focused on the alginate-Ca^{2+} system and tested the injection of different concentrations of ions to 1 wt.% polymer. We conducted time sweep experiments ($\gamma = 3\%$, $\omega = 1$ rad/s) at 25 °C using the KINEXUS Ultra+ rheometer. The novel setup can successfully record *in situ* the fast gelation from the early stages. G′ and G′′ increase sharply in the beginning. However, at longer times, a quasi-steady state is observed as the structural networks created and the ions diffuse slowly to alginate. Also, the temporal development of tan(δ) can be well described by $\tan(\delta) = 1/(\tau\delta)$, which corresponds to a single Maxwell model with a single relaxation time τ. By increasing the concentration of ions, matching results of tan(δ) were observed, at 1000 s of the reaction, due to the similar relaxation times of the gel structures because of the balance between the diffusion of ions and the formation of new linkages.
Finally, this setup can be used to study the kinetics of similar systems whose gelation depends on a well-controlled process and can be applied in industry.

[1] Besiri, Goudoulas, Germann, Carbohydr. Polym., 2020, 246, 116615

Thursday 14:20 Virtual / Track 6 ER24

Magnetorheology in precession fields: from uniaxial DC to rotating AC fields

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Magnetorheological (MR) fluids have traditionally been studied under uniaxial DC fields. In this case, suspended magnetizable particles become magnetized and subsequently form elongated anisotropic structures aligned with the field. This results in dramatic changes in the rheological response and the appearance of a yield stress. Beyond static fields, MR fluids have also been studied under rotating AC fields to examine the aggregation dynamics but their rheological behavior remains unexplored. In this communication we report, for the first time, the rheological behavior of MR fluids in the gap between uniaxial DC and rotating AC fields changing the precession angle and keeping the field strength constant. A new Mason number (Mn) is defined and both rheomicroscopy and particle-level simulations are carried out under the presence of magnetic fields to correlate the particle microstructure with the macroscopic rheological performance.

For low angle precession fields the MR response is optimized as linear structures are fortified and preserved during the field transitions. Low angle precession fields are observed to promote lateral chain coalescence, which in turn strengthens their response to chain deformation under applied shear. For large angles of precession and high Mn time-averaged interactions encourage particle migration into layers, which often results in weaker segmented structures following a field transition.

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Thursday 14:40 Virtual / Track 6 ER25

OrthoChirp: Fast spectro-mechanical probing of transient microstructural evolution during shear

Christian Clasen[1], Gareth H. McKinley[2], Michela Geri[2], Joshua David John Rathinaraj[2], and Jan Hendricks[1]
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Shear-induced microstructural changes in complex fluids as diverse as food gels, consumer products and fracking fluids are governed by fast internal time scales that are of relevance to material processing operations and often impact the final material properties. To gain insights into these time scales, traditional mechanical spectroscopic techniques such as Small Amplitude Oscillatory Shear (SAOS), and more recently MAOS/LAOS, have been proven to be useful. However, probing such spectra and their transient evolution during shear is challenging: firstly, time-evolving microstructures complicate the measurement of discrete mechanical spectra, since the material evolves or "mutates" on time-scales comparable to the time scale of the measurement. Secondly, if both modes of deformation are parallel to each other, cross-coupling of the steady- and oscillatory flow fields can lead to unexpected changes in the material measurements (such as apparently negative values of the elastic modulus). To address both of these challenges, in the present work, fast exponential chirp signals are superimposed orthogonally onto materials undergoing steady shearing deformation. The utilization of multispectral chirp signals reduces the measurement time required to acquire a frequency spectrum (as compared to traditional discrete frequency sweeps), whilst the orthogonal driving decouples the steady flow field from the oscillatory shear field. We demonstrate the utility of this orthogonal chirping using physically-associated alginate solutions, for which the shear- rate-dependent orthogonal moduli can be well-described by a fractional Maxwell liquid (FML) constitutive model. The capabilities of this combined technique (the 'OrthoChirp') pave the way towards better understanding of shear-rate-dependent viscoelastic properties, in particular for weakly-associated physical gels undergoing (relatively) fast transient evolution.

Thursday 15:40 Virtual / Track 6 ER26

Custom 3D printed vane-like geometries for more accurate rheometry of yield stress fluids

Crystal E. Owens[1], Emad Chaparian[2], Jeffrey R. Hesslink[1], A. John Hart[1], and Gareth H. McKinley[1]
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A major challenge of rheometry is to measure true material properties. However, the tools used can strongly influence results, especially for history-sensitive and slipping materials including most yield stress fluids. Errors from slip, shear banding, tool insertion-induced rejuvenation, and inhomogeneous deformation may easily be hidden by test results reported only as bulk values, putting the burden of good experimental technique and interpretation on experimentalists. While the 4-bladed vane often provides an adequate compromise between quasi-rheometric flow kinematics and robust measurements, it is imperfect.

We introduce a modified vane-bob hybrid we call the dodeca-roto-dendron. Twelve dendritic fingers grip the fluid, extending in a finite fractal pattern from the rotor's core axis. This provides a more cylindrical yield/shearing surface than the 4-arm vane, while the use of concave internal voids simultaneously reduces eddying of fluid internal to the vane perimeter, expanding applicability to less viscous fluids. We describe the use of the dodeca-roto-dendron to measure yield stress and flow curves. This tool provides an accuracy within 3% of roughened cone-and-plate reference measurements and expanded range compared to 4-arm vanes. We further report flow-field information for fluids having different yield stress levels, using adaptive finite element/augmented Lagrangian method simulations with varied Bingham numbers. We support these results using a custom 3D printed cup with an integrated mirror for flow visualization. The particular fractal structure was developed for azimuthal shear stress homogeneity, though we show that the shear field and resulting measured torque are remarkably insensitive to the tool's internal structure, allowing greater design freedom and room for further innovation. Finally, we briefly introduce a low-cost handheld 3D printed rheometer that is capable of measuring yield stresses of fluids without a cup, thus perfectly eliminating slip at the outer wall.

Symposium CF

Complex flows

Organizers: Rossana Pasquino and Francisco Galindo Rosales

Thursday 14:00 Virtual / Track 7 CF14

Injection of a yield stress fluid into a lighter Newtonian fluid: on facilitating an unstable stratification

Abdallah Ghazal and Ida Karimfazli
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Off-bottom cement plugs are commonly used in oil well abandonment operations. In such application, heavy cement slurry is commonly injected in cased wells that are otherwise filled with lower density wellbore fluids. A successful placement operation relies on the accumulation of the cement slurry at the target position, on a layer of the wellbore fluids. The favorable outcome is thus likely to be prevented by the buoyancy-driven displacement of the cement slurry. We develop an idealized model of the injection process to investigate the hydrodynamic events following the onset of injection. The goal is to investigate the feasibility and to reveal the underlying mechanisms of off-bottom plug placement. The cement slurry and wellbore fluids are modelled as yield stress and Newtonian fluids, respectively. We consider the injection of a yield stress fluid in a vertical two-dimensional channel, where the injection tube is concentric with the casing. We illustrate that the formation of a mixed layer beneath the injection point leads to the accumulation of the yield stress fluid around the target position. We consider a wide range of Peclet numbers to characterize the role of diffusion. We identify highly diffusive and advective regimes as the two extreme flow regimes and provide a mechanistic description of the different scenarios for successful placement.

Thursday 14:20 Virtual / Track 7 CF15

Free convection of carbopol microgels: the limitations of viscoplastic models

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A fluid with a yield stress (YSF) flows if the applied shear stress suppresses a threshold value called the "yield stress". Viscoplastic models (VPM) are a family of constitutive laws most commonly used for theoretical and computational studies of YSFs. One of the primary assumptions in VPM is the rigidity of YSFs below the yield stress. If the yield stress is exceeded, VPM describe the material behaviour using a shear rate-dependent viscosity. It follows that (i) the buoyancy stress must exceed a threshold value for steady free advection in YSF and (ii) the onset of advection may be delayed by a finite time that increases with the yield stress (see e.g. [1]).

In order to assess these theoretical predictions, we conduct an experimental investigation of the free convections of carbopol microgels in a cavity with differentially heated sidewalls. The fluid is initially motionless and at a uniform temperature. We use time-resolved particle image velocimetry along with thermochromic liquid crystals to characterize the development of the velocity and temperature fields. We illustrate that indeed a threshold ratio of the buoyancy and yield stresses exists, below which the steady-state is motionless. The development of the motionless or advecting steady states, however, has marked differences with the predictions based on VPM. We reveal the immediate development of motion in the fluid at the start of all experiments regardless of how the buoyancy stress compares with the yield stress and propose possible interpretations of our observations.

[1] Karimfazli, I., and I. A. Frigaard. "Flow, onset and stability: Qualitative analysis of yield stress fluid flow in enclosures." Journal of Non-Newtonian Fluid Mechanics 238 (2016): 224-232.

Thursday 14:40 Virtual / Track 7 CF16

Viscoelastic fluid flow in microporous media

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The importance of the flow of viscoelastic fluids through porous media in the chemical, biological, and oil industries has led to the topic receiving significant attention from researchers over the past decade. Although progress has been made in this time, the scarcity of comprehensive rheology data as well as the limitation of measurement techniques has restricted most of the studies to average macroscopically measurable flow quantities like porosity, permeability, and pressure gradient. As a result, the subject remains incompletely understood. Here we describe an experimental investigation of the flow of flexible polymer solutions through a distinctive micro-porous structure (typical pore sizes of 500 microns) with the primary focus on the interaction of the viscoelasticity of the working fluid (which is characterized both in shear and extension) with the micro-porous structure. In particular, we relate the bulk flow properties to measurable rheological parameters, demonstrating that a key parameter in estimating the pressure drop through the porous media (for a variety of polymer types, concentrations, solvents, molecular weights, and states of degradation) is the extensional relaxation time. A Weissenberg number (Wi) is calculated as a product of this extensional relaxation time and the nominal shear rate in the flow. Results, suitably normalized with Newtonian pressure-drop data, show a critical Wi of roughly 0.01 where all working fluids reveal the onset of elastic dominance over viscous forces as the flowrate increases. Such a low critical value of Wi is due to the estimate of a nominal shear rate based on pore size, which severely underestimates the maximum shear rates within the complex pore structure. However, this implies that, although the flow through porous media is known to be a complex combination of both shear and extensional flow, the extensional effects are of primary importance in the context of viscoelasticity.

Thursday 15:40 Virtual / Track 7 CF17

Impact of the wetting length on flexible blade coating

Marion Krapez[1], Anaïs Gauthier[1], Jean-Baptiste Boitte[2], Christophe Kusina[2], Danielle Le Verge[2], Angelina Roudot[2], Hamid Kellay[3], Jean-François Joanny[4], and Annie Colin[1]

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We study a common industrial problem: the spreading of a fluid, Newtonian or complex, by a deformable blade, which is also paradigmatic of elasto-hydrodynamic interactions. This question has been seen in the light of an elasticity-capillarity analogy, and a parallel with dip coating experiments was proposed to predict the deposited film thickness for a Newtonian fluid [1]. To do so, the liquid reservoir was always considered as infinite. Here, we consider the case of a finite reservoir of liquid, emptying as the liquid is spread, a situation corresponding to a large majority of everyday situations, such as the spreading of paint on a wall, or cream on the skin. We evidence the role of a central variable: the wetting length lw, which sets a boundary between the wet and dry parts of the blade. We show that the deposited film thickness depends quadratically with lw. We study this problem experimentally and numerically by integration of the elasto-hydrodynamic equations, and propose a scaling law model to explain how lw influences the spreading dynamics. We finally extend the model to complex fluids, and in particular shear thinning fluids, once again highlighting the importance of lw.

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Thursday 16:00 Virtual / Track 7 CF18

On the role of Weissenberg and Deborah Numbers in the scission of semidilute unentangled polymer solutions in fast transient extensional flow

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Scission of polymers results in large viscosity losses, which is major concern in different industrial applications. In this work we study the relevance of the two characteristic numbers: Weissenberg and Deborah number for polymer scission. Weissenberg number defines scission process to be a critical stress criterion (instantaneous process) and gives the actual force required to break the C-C bond. While a Deborah number, defines the scission process to be an energy activated process; when a force is applied to stretch the polymer the energy barrier required decreases (gradual process). To understand the most relevant criterion for scission, semi-dilute unentangled polymers solutions are injected through specially-designed microfluidic hyperbolic contraction geometries with Hencky strains ranging from 1.4 to 4 units. The ratio of the pressure drop of the polymer solution to that of the (Newtonian) solvent has a maximum when plotted as function of flow rate. This maximum results from the competition between polymer extension and scission. For a given Hencky strain, the maximum in pressure drop ratio curve occurs for a fixed Weissenberg number. With increase in Hencky strain the maximum in pressure drop ratio curve occurs for smaller Weissenberg number. At the maximum in pressure drop ratio, the Deborah number is exponentially related to the strain rate. From the equivalence with the TABS model, rate of scission has a similar exponential dependence with the force required to break the polymer chain, we suggest scission process to be an energy activated mechanism. Furthermore, scission is also studied from the double passages. A scission model is proposed to predict the quantity of scission in the first passage by characterizing the pressure drop ratio of the second passage. This scission model consists of scission exponent b, which defines the broadness of transition from no scission to scission dominated regime and is a function of the Hencky strain.

Thursday 16:20 Virtual / Track 7 CF19

Thermo-structural behavior of sepiolite clay dispersions: a comparative study based on thermal cycling test

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Clays are the main components of various complex fluid systems used in different industries. Structural deformation of utilized clay under the effect of temperature has been widely considered in some application area. This study involves the thermo-structural behavior of clay dispersions as the main components of drilling fluid subjected to thermal cycle while circulating in the wellbore. Various experimental methods, setups, and procedures have been employed in literature to analyze the thermal stability, alteration, and degradation of colloidal dispersions. This study is an attempt to monitor the thermo-structural behavior of sepiolite clay dispersions under a thermal cycling test. Four types of sepiolite clay were collected directly from four different beds located in Sivrihisar, a district of Eskisehir Province in the Central Anatolia region of Turkey. Large pieces of collected Sepiolite clays were exposed to some physical treatments (rotary grinding and high-speed dynamic air classifier) to obtain finer grain sizes (<75 µm). Clay dispersions with distilled water were prepared using powdered sepiolite clays and a commercial bentonite clay (Wyoming bentonite) as the API reference clay by means of the high shear mixer. Discovery Hybrid Rheometer (DHR-II) was used to apply the thermal flow ramp cycling test using a pressure cell unit with a conical rotor. Five thermal cycle tests from 25 °C up to 150 °C were carried out

to simulate wide ranges of temperature variation. Graphical analysis based on relative changes between the viscosity value in each cycle and the viscosity value in the initial cycle was made to determine the degree of the structural changes in clay dispersion samples. Findings revealed that dispersion samples prepared with sepiolite clays provided exceptional thermo-structural stability compare to Wyoming bentonite dispersion. The usage of the sepiolite clay as the main component of drilling fluid could be an efficient alternative, particularly in hostile drilling conditions.

Symposium MS

Modelling and simulations

Organizers: Natalie Germann and Daniel Read

Thursday 14:00 Virtual / Track 8 MS32

Modeling the flow behavior of catalyst inks for PEM fuel cells by an evolutionary algorithm

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The catalyst coated membrane represents the heart of a polymer electrolyte fuel cell (PEMFC) and is produced by directly applying a catalyst suspension on the membrane or a decal transfer foil. Understanding the rheology of catalyst inks is crucial to optimize the printed microstructure of the catalyst layer and hence the performance of the fuel cell. The suspension consists of platinum on carbon powder, ionomer dispersion (perfluorosulfonic acid ionomer) and solvents. Its rheology is directly affected by various material properties of all ink components. Therefore, measuring the flow curves represents a suitable tool for quality control at the beginning of the production line. In this study, we investigate the influence of carbon to solvent ratios with and without ionomer as well as different types of ionomers (equivalent weight variations) on the inks flow behavior. Moreover, we compare low surface carbon (VulcanXC72R) with high surface carbon (Ketjenblack EC300J) for all ink variations. A rotational rheometer with TwinDrive technology is used to analyze a total of 20 different ink recipes. Four measuring profiles are applied to characterize the dynamic viscosity and yield stress in rotational mode and the viscoelastic behavior by amplitude sweep. Further, three interval thixotropy tests are conducted to investigate the transient flow behavior during oscillation. The collected data is fitted by an evolutionary algorithm to common models for Non-Newtonian flow, like Power Law, Cross Power Law, Bird-Carreau and Herschel-Bulkley models. Thereby, determined parameters are then linked to the ink component and their material properties. The resulting correlations and database represent the first step towards designing desired flow behaviors for coating processes, hence optimizing the production process, as well as predicting the ink microstructure by only knowing material properties and proportions of the catalyst ink ingredients.

Thursday 14:20 Virtual / Track 8 MS33

Rheology of suspensions of bubbles in an elastoviscoplastic fluid

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The oscillatory shear flow of Newtonian bubble suspensions in an elastoviscoplastic (EVP) fluid is simulated using a second order finite-difference method and level set method. The governing equations are advanced in time using a linear, two-step Adams-Bashforth method. The constitutive equation of Saramito [1] is used to model the extra stress tensor contribution of the EVP to the momentum equation, which models the EVP as a Kelvin-Voigt viscoelastic solid in its unyielded state and an Oldroyd-B viscoelastic fluid in its yielded state. The material properties for the modeled EVP (aqueous solution of 0.07% w/w Carbopol 940) are fitted to data of oscillatory shear experiments found in literature. An isotropic kinematic hardening model is incorporated for the EVP which has been shown to predict the low strain amplitude viscous response that this Carbopol solution has been shown to exhibit. 3D, direct numerical simulations and parameter sweeps of the gas volume fraction and the Capillary number are performed to investigate the effect that inclusions of deformable bubbles have on the rheology of the investigated suspensions, namely the effect on the dynamic moduli, G' and G''. This is computed using the leading harmonics of the Fourier series expansion: $\tau=\gamma_0[G'\sin(\omega t)+G''\cos(\omega t)]$. It is found that the results are in qualitative agreement with experimental results found in literature of bubble suspensions in yield stress fluid models that comprise concentrated emulsions, in that deformable bubble inclusions lead to a softening of the suspension, thus a decrease in the dynamic moduli. Parameter sweeps of the Weissenberg and Capillary numbers are also performed for the case of a single droplet in the same EVP under simple and oscillatory shear flow conditions to investigate their effect on the stress fields.

[1] P. Saramito, "A new constitutive equation for elastoviscoplastic fluid flows," Journal of Non-Newtonian Fluid Mechanics, vol. 145, no. 1, pp. 1-14, 2007.

Thursday 14:40 Virtual / Track 8 MS34

A simple continuous viscoelastic model for yield stress fluids

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A new model for viscoplasticity is presented and compared to the transient nonlinear rheology of a model yield stress fluid. The model parameters are determined by the linear viscoelastic and steady shear responses obtained from frequency sweep and flow curve measurements. The smooth overshoot in the loss modulus that is typically observed in amplitude sweeps of yielding materials is accurately predicted, including the smooth transitions recently observed in terms of recoverable and unrecoverable component strains [1]. The model contains a rate-dependent relaxation time, which is shown to give rise to a constant apparent yield strain at low rates and a rate-dependent apparent yield strain at higher rates. The model accurately predicts a bifurcation in the viscosity and avalanche dynamics under stress-controlled protocols. The model is expressed as a single differential equation that makes no distinction in the physics that governs the behavior of the yielded and unyielded states and therefore constitutes a simple tool for the study of yielding.

[1] Donley et al, PNAS 117 (36) 21945-21952 (2020)

Thursday 15:40 Virtual / Track 8 MS35

Mesoscopic modeling of the Endothelial Monolayer and its response to shear-induced blood flow

Konstantina Psaraki, Vlasis Mitsoulas, Yannis Dimakopoulos, Stavros Pavlou, and John Tsamopoulos
Chemical Engineering, Fluid Mechanics and Rheology, University of Patras, Patras, Greece

Endothelial cells form the basic barrier between blood vessels or capillaries and tissue [1]. Shear stress, which is the frictional force developed by blood stream above the endothelium, can elicit various responses like cell deformation, cytoskeletal rearrangement, and activation of signaling pathways [1]. Although the precise mechanisms of mechanical-chemical coupling in ECs exposed to shear-stress are not fully understood, the biochemical cascade for nitric oxide (NO) overproduction and calcium ions (Ca^{2+}) dynamics are linked to many harmful effects such as inflammations and induction of apoptosis [2]. This implies that we should deeply investigate the structural and chemical responses of endothelial cells under shear experiments and develop reduced biochemical models to provide accurate predictions with the minimum possible input. We present a new mesoscopic model for the response of endothelial monolayer to shear-induced blood flow, accounting for the fluid-structure interaction phenomena between the deformable endothelium and blood plasma. We employ an advanced Finite Element Method, while introducing a poroelastic constitutive model for the rheological characterization of the cytoplasm. By modeling the cytoplasm as a biphasic medium, the mesh corresponds to the solid phase, forming a structure of solid net. We expect that the elasticity will differ from other works adopting hyperelastic models for the cell mechanics. We evaluate the rheological properties of the cell by implementing a benchmark compression experiment introduced by Caille et al.[3]. We conclude that under start-up shear the blood flow strongly affects not only the endothelial cell's structure but also leads to a slight uplift of the nuclear domain.

[1] Fels J, Jeggle P, Liashkovich I, Peters W, and Oberleithner H. Cell and tissue research 355: 727-737 (2014).
[2] Pinton P, Giorgi C, Siviero R., et al. Oncogene 27: 6407-6418 (2008).
[3] Caille N, Thoumine O, Tardy Y, and Meister JJ. J Biomech. 35(2):177-87 (2002).

Thursday 16:00 Virtual / Track 8 MS36

Numerical simulation of viscoelastic droplet formation in dripping regime

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Droplet formation of viscoelastic fluids is of paramount importance for numerous industrial applications such as 3D-printing and coating technology. A profound understanding of the complex topological changes during the capillary driven thinning and pinch-off is essential for the accurate prediction of such processes. In the present study, a computational fluid dynamics model is employed to investigate different stages of the droplet formation of viscoelastic fluid in dripping regime. The numerical simulations are carried out using an axisymmetric domain and the interface tracking is performed by using level-set model. The Oldroyd-B constitutive model is employed to consider the viscoelasticity. The accuracy of the CFD model is first validated against the available experimental data. Furthermore, the influence of Deborah number and Ohnesorge number on the interface evolution during the necking stage is investigated. In addition, the thinning behavior and the flow characteristics in inertio-capillary and elasto-capillary regimes are explored based on the obtained CFD results.

Thursday 16:20 Virtual / Track 8 MS37

Die shape optimization for extrudate swell using feedback control

Michelle M. Spanjaards, Martien A. Hulsen, and Patrick D. Anderson
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Extrusion is a widely used process to create products with a fixed cross-sectional profile. Many applications require cross-sections of complex shapes, where the dies contain sharp corners. Common requirement on the extrudate is dimensional precision. The dimensions of the extrudate are highly influenced by extrudate swelling. The swelling process involves complex dynamics influenced by many parameters, such as viscoelasticity. Therefore, the optimized shape of a die, to obtain an extrudate with desired dimensions and shape, is now often obtained through trial-and-error.

We developed a transient 3D finite element model, to predict extrudate swelling for extrudates containing sharp edges. This model describes the corner lines of the domain separately to obtain the positions of these lines in the two swell directions. A 2D height function is used to describe the free surfaces of the extrudate, using the positions obtained from solving the material lines to expand the domain of the height function [1]. A convergence study of a benchmark problem is performed to validate the model.

A novel approach to solve the inverse problem of three-dimensional die design for extrudate swell is developed, using a real-time active control scheme. To this end, a feedback connection between the corner-line finite element method and the controller is envisioned. In this talk we show the validity of this method by showing optimization results for 2D axisymmetric extrusion flows of a viscoelastic fluid for different Weissenberg numbers. In 3D we first give a proof of concept by showing the results of a viscous fluid exiting dies with increasing complexity in shape. Finally, we show that this method is able to obtain the desired extrudate shape of extrudates of a viscoelastic fluid for different Weissenberg numbers and different amounts of shear-thinning.

[1] M.M.A. Spanjaards, M.A. Hulsen, P.D. Anderson. Journal of Non-Newtonian Fluid Mechanics, 270:79-95, 2019

Symposium PM

Polymer melts and composites

Organizers: Maria Teresa Cidade and Juan de Vicente

Thursday 14:00 Virtual / Track 9 PM40

Investigation of rheological and mechanical properties of tailor-made POM-POM model systems

Marie-Christin Röpert, Valerian Hirschberg, and Manfred Wilhelm
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In this work, a series of Polystyrene (PS) based model systems with a POM-POM architecture was synthesized by the combination of anionic polymerization technique and grafting-onto method to investigate the molecular origin of rheological and mechanical properties.

The POM-POM topology is defined by four main molecular parameters: (I) the distance between the two stars / POMs, (II) the number of side chains per POM and (III) their length and furthermore, (IV) if more than one chemically identical monomer is used, i. e. (block) copolymers, the chemical composition of the backbone and side-chain. Investigating the rheological properties and correlating them to the molecular topological parameters requires controlled synthesized and well-characterized polymer model architectures.

The tailor-made POM-POM model systems used in this study have a constant backbone length, whereas the length and number of the side chains are varied. Shear and extensional rheological data of these POM-POMs were investigated in the framework of zero shear viscosity (η_0) and strain hardening factor (SHF) and correlated with the molecular structure.

First experiments revealed that the length of the side chains stretches the rubbery regime for a similar backbone up to 8 decades, and drastically increases the zero shear viscosity by over a factor of 500 compared to the sidechain. In the terminal regime, G' and G'' are parallel with a constant slope of around 0.6. Moreover, the POM-POM topology highly improves the fatigue lifetime of polymers. PS POM-POMs topology has shown to be extremely promising compared to linear PS, as in torsion the deformation during breakage was exceeded by 60 % and the fatigue properties by more than a factor of ten. Also, the material properties changed from brittle to ductile.

Thursday 14:20 Virtual / Track 9 PM41

Understanding the effect of recycling on the rheology and processability of polyethylene blends

Sylvie Vervoort
Dow Benelux, Hoek 4542 NM, The Netherlands

Plastics recycling is high on society's agenda nowadays. Recycled polyethylene (rPE) is typically a mix of different types of polyethylene (low density (LDPE), linear low density (LLDPE), some high density (HDPE)) contaminated with small amounts of other polyolefins such as polypropylene. The polymers in such mix are reprocessed together several times when going through multiple recycling and re-use steps. A certain level of degradation can be expected. However, it has not been studied systematically how recycling affects the PE mixture and more specifically, how this affects its flow behavior, one of the key properties to enable transformation into a valuable recycled product. A better understanding of these effects can be an enabler for more efficient integration of recycled PE in the material stream. To this purpose, a model plastic film formulation composed of an LDPE/LLDPE blend was studied through multiple processing steps. At each pass, the polymer blend is subject to thermal, mechanical and oxidative strain. All these strains have the potential to alter the polymer chains. The changes in shear and extensional flow behavior will be presented and the consequences of recycling on processability and optical properties of a plastic film will be discussed. These will also be related to changes at the molecular level.

Thursday 14:40 Virtual / Track 9 PM42

Extrusion challenges in fused filament fabrication: experimental investigation of the dynamic behavior of the extrusion flow

Paola Fanzio[1], T Schuller[2], and Francisco J. Galindo-Rosales[3]
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Fused Filament Fabrication (FFF) is the most versatile and rapidly growing additive manufacturing technology. In a typical process, a thermoplastic filament is fed into the machine via a pinch roller mechanism and melted in a heated liquefier with the solid portion of the filament acting as a piston to push the melt through a nozzle. Movement of the print head allows to deposit the material in specific locations, thereby layer-by-layer building of custom 3D geometries.

Thanks to the wide variety of available materials, wide range of operating length scales and the low cost, the field of applications is remarkably broad, spanning from architecture modelling to engineering. Recently, a growing interest in local-digital manufacturing and the need of building functional prototypes and tools is pushing the development of 3D printers with higher performances. However, there are still gaps of knowledge that need to be overcome for the development of the next generation of printers. For instance, research on the extrusion process and its influence on the properties of 3D printed parts is of paramount importance for the control of the printing process.

In this presentation, experimental data on the measurement of the die-swell exhibited by the polymer melts at the exit of the print-head by means of a high speed camera is presented. Those measurements allow to characterize the transient behavior of the extrusion flow in a free air extrusion setup. On the other side, in a 3D printer, the molten polymer is deposited on a build surface. The deposition dynamics is evaluated by measuring the width of lines deposited on a glass build plate at different extrusion flows. Results show that the two processes are directly linked, opening up new possibilities to characterize, predict and control the 3D printing process.

Finally, some open challenges related with FFF will be presented to underline the importance of the control of the extrusion process and the polymer rheology in order to increase the printing quality.

Thursday 15:40 Virtual / Track 9 PM43

Effect of non-solvent addition in dopes on rheology and coagulation kinetics of poly-(o-aminophenylene)naphthoylenimide solutions

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Production of thermal and heat resistant PNBI (polynaphthoylbenzimidazole) fibers by ecological friendly methods is possible through previous obtaining of poly-(o-aminophenylene)naphthoylenimide (PANI-O) precursors. The PANI-O could be synthesized in organic solvents (DMSO or NMP) which is more convenient compared with sulfuric acid used for PNBI synthesis. Solubility and rheological parameters of PANI-O solutions in organic solvents are changed in time due to reactions of intramolecular cyclization and polymerization. One of the technological tasks for PANI-O solutions is controlling and fast measuring those parameters for the preparation of spinning dopes. Fiber spinning from these dopes is possible only via the wet process, and coagulation bath composition is the most important for defectless fiber production. As usual, the multicomponent coagulant composition and suitable solution viscoelastic properties are responsible for the stable fiber production process.

We suggest a new method for controlling the rheological properties of dopes by introducing non-solvents in PANI-O ⁄ NMP solutions. The wide concentration range was investigated by polymer and non-solvent. It was shown non-solvent (water or ethanol) addition to the polymer solutions makes it possible to obtain solutions in the wide range of viscoelasticity from Newtonian liquids to shear-thinning or yield stress appearing that accompanying by reducing the activity of the solvent and accelerating the coagulation process. The last one is initiated by the same coagulant and minimizes the number of macro defects in fibers. The combination of parameters under investigation made it possible for the first time to develop new principles of modifying polymer dopes for wet spinning and finally to obtain qualitative heat-resistant PNBI fibers [1].

The study was financially supported by Russian Foundation for Basic Research (grant # 18-29-17062 mk).

[1] doi:10.3390/polym12112454

Thursday 16:00 Virtual / Track 9 PM44

Next-generation layer multiplication co-extrusion: tubes, bags, pipes and bottles

Joao Maia, Erik Steinmetz, and Tyler Schneider
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Layer multiplication co-extrusion is a process of substantial academic interest and achievement and one of proven industrial application. The industrial adoption of the process has primarily been in the realm of specialty and advanced products in film geometries for applications such as UV control and strength in windows, decorative coatings for marketing and aesthetics, and barrier applications for control of packaging environments. Recently, our group expanded the processing realm into high viscosity and high elasticity ratios, as well as to annular geometries and has begun to demonstrate the functional application of such products. In addition to presenting this novel technology, we will present results on three different systems/application products. First, mechanical strength improvements, including increased burst resistance, of layered pipes are demonstrated with the implementation of the technology of die head rotation in conjunction with layer multiplication. Second, the translation of this technology to the area of extrusion blow-molding is demonstrated by the creation of the first ever bottles containing up to 131 layers. Finally, novel layered foam tubing that could show potential strength improvements to light weight piping has also been developed and will be presented.

Thursday 16:20 Virtual / Track 9 PM45

Adhesive tape peeling over soft micro-textured substrates

Hélène Piot-Durand[1], Stéphane Santucci[1], and Loïc Vanel[2]
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The simultaneous control of the adhesion strength and the detachment dynamics of soft adhesive materials is a key improvement lever for gluing and sealing applications in various industrial domains. The most common approach to optimize adherence and debonding processes involves chemical modifications of the polymeric adhesive layer and/or of the substrate interface. We propose to investigate another possibility by introducing physical modifications of the substrate, changing its topography, its elastic properties and interfacial energies. Therefore, we have performed a thorough experimental study where a pressure-sensitive adhesive tape (PSA) is peeled from a transparent substrate at a constant imposed velocity over a very wide range (µm/s to m/s). For largest peel velocities, the detachment front of our PSA presents usually a "stick-slip" propagation, alternating periodically slow and fast phases, and accompanied by drop in the effective adhesive energy. Taking advantage of the transparency of the substrate, we can visualize the detachment process and simultaneously monitor the peeling force. We could prepare our own substrates using different materials: glass and Plexiglas (PMMA) plates, PDMS layers of various thicknesses and elastic moduli (either adsorbed at an interface or in bulk), UPVC films (corresponding to the adhesive tape backing), leading to different levels of interfacial energies and stiffness. We could produce micro-textured surfaces using either a micro-milling machine or lithography techniques. We opted to pattern regular grooves of a few microns deep and wide regularly spaced of a few microns in either PDMS or PMMA samples.

Our first results show that the combined deformation of the substrate and adhesive enhance the adhesion strength and affects the detachment front dynamics by shifting the velocity threshold of appearance of the "stick-slip" instability. We also demonstrate the possibility of controlling the microscopic instability of the detachment through the substrate texture.

Symposium IR

Interfacial rheology, emulsions and foams

Organizers: Anniina Salonen and Nikolai Denkov

Thursday 14:00 Virtual / Track 10 IR32

Understanding the role of interfacial rheology on electrocoalescence

Alexandra Alicke and Jan Vermant
Department of Materials, ETH Zürich, Zurich, Switzerland

The stability of water-in-oil emulsions can pose serious challenges in the transportation and separation of crude oils. The high stability of these emulsions has been mainly attributed to the presence of asphaltenes at the interface, although the precise mechanisms by which they act are not fully understood. Being one of the more polar fractions in crude oils, asphaltenes are surface active and strongly adsorb at the o/w interface, and recent results suggest that these are not very efficient in lowering interfacial tension but rather impart significant mechanical stresses [1]. Indeed, understanding the fundamentals of the stabilization mechanisms in emulsions is paramount to design effective destabilization processes. Different destabilization strategies are used in oil fields, such as the use of demulsifiers and application of an external electric field. Frequently both approaches are combined and seem to be more effective, although the exact underlying mechanisms by which they enhance coalescence still needs to be clarified. Hence, our goal is to understand how the interfacial properties affect the stability of these systems at a microscale, namely by looking at the thin liquid film of continuous phase that drains when two droplets approach. To this end, we use the thin film balance technique combined with E-fields to study the drainage and rupture of these films. Asphaltene films show viscoplastic response with a high stability against electrocoalescence, except when combined with demulsifiers. We also carry out experiments with surfactant films to gain a better understanding of the fundamentals of this phenomenon. We observe that the critical voltage required for rupture depends mainly on film thickness, with highly localized thinning in mixed asphaltene/demulsifier systems. With these results, we can obtain important insights into the mechanisms leading to coalescence with the potential to provide more effective and energy-efficient approaches to destabilize these emulsions.

[1] Alicke et al, Langmuir (2020)

Thursday 14:20 Virtual / Track 10 IR33

Influence of thin films rheology in coalescence

Laura M. Torrès, Isabelle Hénaut, and Christine Dalmazzone
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The mechanisms of coalescence is of huge importance in the process of soft matter and divided materials such as emulsions and foams. It controls their stability and their final properties in many applications including cosmetics, food engineering, energy, biotechnology etc. It has a significant influence in wastewater treatment. Actually oil removal relies on gravitational methods that are favored by coalescence. In Enhanced Oil Recovery, water treatment is all the more challenged by residual polymers and surfactants that constitute complex physicochemical systems. The objective of this work is to characterize the mechanisms involved in the coalescence in the flotation process. To do so, drainage and rupture steps of thin films between an oil droplet and a gas bubble were investigated. The thin films were composed either of biopolymer or of synthetic polymer in dilute and semi-dilute regime concentrations. This diversity of samples allows a large range of rheological behavior, intrinsic viscosity and gyration radius. It was shown that extensional properties have generally the most impact on thin films rupture. Flow properties of the thin films were addressed using rheometers and microfluidic devices. A dedicated set-up enabled to film with a high speed camera the coalescence of an oil droplet with various interfaces. Spreading of the oil at the interface was also recorded and analysed. In addition, macroscopic experiments were performed with a lab flotation column. This whole set of experiments demonstrates how small scale phenomena such as the ones involved in coalescence can govern macroscopic ones in processes.

Thursday 14:40 Virtual / Track 10 IR34

Confined tube flow of emulsions: from single droplet deformation to collective rheological behavior

Valentina Preziosi, Giovanna Tomaiuolo, and Stefano Guido
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Droplet-based systems like emulsions are widely used in many relevant industrial applications, such as in the food, biomedical and petrochemical fields. In particular, droplet flow and deformation in microconfined conditions is a topic of relevant importance especially in processes such as the flow in porous media [1] or the flow of red blood cells in microcapillaries[2]. Although the literature contains many papers regarding the behaviour of droplet-based systems in static conditions, the effect of flow in microconfined conditions has been mostly investigated by theoretical models, while still lacking from the experimental point of view [3,4]. Such problem can even result more complicated when one of the two emulsion liquid phase flowing in a microfluidic device is non-Newtonian, and the effect of elasticity and shear rate dependent viscosity have to taken into account. In this work, an overview on emulsion fluid dynamic behavior in microconfined conditions is reported. Starting from the theoretical works reported in the literature, a microfluidic device to measure in situ the interfacial tension of emulsions, by using different surfactants, from droplet deformation under simple shear flow is presented [5]. Moreover, the effect of elasticity on droplet behaviour can be investigated separately from the shear thinning effects by using particular fluids (Boger fluids [6]) exhibiting the viscosity nearly constant with the shear rate. The influence of matrix elasticity on the droplet size distribution and on the formation of a cell-free layer at the wall is also discussed.

[1] A. Perazzo et al., Advances in colloid and interface science 2018, 256, 305
[2] G. Tomaiuolo et al., Soft Matter 2009, 5, 3736
[3] V. Preziosi et al., Chemical Engineering and Processing-Process Intensification 2018, 125, 275
[4] V. Preziosi et al., Soft Matter 2017, 13, 5696
[5] R. D Apolito et al., Langmuir 2018, 34, 4991
[6] V. Preziosi et al., Journal of Rheology 2016, 60, 419

Thursday 15:40 Virtual / Track 10 IR35

Effect of droplet size on the rheology of high internal phase emulsions with adhesive and repulsive droplets

Muchu Zhou and Reza Foudazi
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High internal phase emulsions (HIPEs) can be produced when the dispersed phase volume fraction exceeds 74%. The HIPEs are used in different applications such as food, cosmetics, and templates for producing porous polymers. The concentrated emulsions with adhesive and repulsive droplets have different rheological properties due to the difference in the interdroplet interactions. Nevertheless, the effect of droplet size on the rheological behaviors of the HIPEs with adhesive and repulsive droplets has not been addressed and discussed. Therefore, in the present work, we study the rheological properties such as dynamic moduli and yield stress of the adhesive and repulsive HIPEs with different droplet sizes. Additionally, the scaling of rheological propertied with droplet size and volume fraction is investigated.

Thursday 16:00 Virtual / Track 10 IR36

Interfacial and bulk rheological analysis of oil-in-water emulsions stabilized by custom-synthesized graphene oxide nanosheets

Elnaz Erfanian[1], Milad Kamkar[2], Parisa Bazazi[1], Hossein Hejazi[1], Gerald G. Fuller[3], and Uttandaraman Sundararaj[1]
[1]University of Calgary, Calgary, Canada; [2]University of British Columbia, Kelowna, BC, Canada; [3]Stanford University, Stanford, CA, United States

Nanoparticle-stabilized oil-in-water (O/W) emulsion has drawn great attention from various industries (e.g., cosmetics, food industry, and enhanced oil recovery (EOR)). Due to the dual nature of graphene oxide (GO) nanosheet, i.e., hydrophobic and hydrophilic, it is very effective at stabilizing O/W emulsions. In this work, we provide a systematic study to examine the performance of the custom-synthesized GO nanosheets (at different concentrations) in O/W emulsion stabilization, utilizing interfacial and bulk rheological techniques. The results demonstrate the excellent ability of GO nanosheets, even at extremely low concentration as 0.04 vol.%, in establishing an elastic film at water/oil interface (shear interfacial elastic modulus as high as 1000 mN/m, which is among the highest reported values in the literature at this low concentration of nanomaterial). Bulk viscoelastic properties and morphology of GO-stabilized emulsions were highly dependent on O/W ratio, GO loading, shear history, and preparation method. For instance, at 0.04 vol.% GO, increasing O/W ratio from 1/1 to 2/1 vol/vol resulted in droplet size reduction of almost 20% and the elastic modulus increased fourfold. However, at 0.3 vol.% GO, bulk elastic modulus and average droplet size remained unchanged upon increasing oil concentration. In addition, emulsions after exposing to shear deformation showed higher monodispersity and the droplet size decreased by up to 18%. This study provides a rheological foundation for many applications such as liquid-liquid printing.

Symposium NF

Living and self-assembling systems

Organizers: Daphne Weihs and Jan Vermant

Thursday 14:00 Virtual / Track 11 NF9

Motion of a self-propelled colloid in the vicinity of a giant lipid vesicle

Vaibhav Sharma, Elise Azar, Andre P. Schroder, Carlos M. Marques, and Antonio Stocco
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Self-propelled colloidal particles either living or artificial, possess authentic dynamics when interacting with other objects like passive particles, interfaces or cell membranes [1]. Interaction of these self-propelled bodies with a biological cell membrane plays a crucial role in many important processes such as viral infections, drug delivery along with nano-material toxicity [2]. Here, we experimentally investigate a biologically mimicking system comprising of self-propelled active colloids existing in the neighbourhood of a Giant Unilamellar Vesicle (GUV). For this study, we focus our attention on the motion of a single active particle interacting with isolated GUVs [3]. We noticed that there is negligible interaction between the colloidal particles and the GUVs in thermal equilibrium. However, when self-propulsion is trigged by the catalytic fuel H_2O_2, the colloids exhibit a persistent hydrodynamic attraction [1,4] with the GUV giving rise to various phenomena like a persistent orbital motion around the vesicle boundary along with displacement of GUV during the impact dynamics.

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Thursday 14:20 Virtual / Track 11 NF10

Solute induced jittery motion of self-propelled droplets

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The intriguing role of the presence of solutes in the activity of a self-propelling droplet is investigated. A system of self-propelling micron-sized 4-Cyano-4'-pentylbiphenyl (5CB) droplets in an aqueous solution of tetradecyltrimethylammonium bromide (TTAB) as surfactant is considered. It is shown that the addition of glycerol causes the active 5CB droplet to exhibit a transition from smooth to jittery motion. The motion is found to be independent of the droplet size and the nematic state of 5CB. Analogous experiments with Polyacrylamide (PAAm), Polyvinylpyrrolidone (PVP), and Polyvinyl Alcohol (PVA), as solutes, confirm that such a transition cannot merely be explained solely based on the viscosity or Peclet number of the system. We propose that the specific nature of physicochemical interactions between the solute and the droplet interface is at the root of this transition. The experiments show that the time-scales associated with the influx and redistribution of surfactants at the interface are altered in the presence of solutes. Glycerol and PVP significantly enhance the rate of solubilization of the 5CB droplets resulting in a quicker re-distribution of the adsorbed TTAB molecules on the interface, causing the droplet to momentarily stop and then restart in an independent direction. On the other hand, low solubilization rates in the presence of PAAm and PVA lead to smooth trajectories. Our hypothesis is supported by the time evolution of droplet size and interfacial velocity measurements in the presence and absence of solute. Overall, our results provide fundamental insights into the complex interactions emerging due to the presence of solutes.

Thursday 14:40 Virtual / Track 11 NF11

Rest time effects on the nonlinear rheology of entangled supramolecular polymers

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The effects of rest time between consecutive steady shear flow experiments have been documented both experimentally and computationally for linear entangled polymers. The test consists of shearing with constant rate until steady state is reached at a given strain, then allowing the system to rest for a specific time, repeating the test and so on. According to the Doi-Edwards model, the recovery time for the stress peak in the repeat test should be the same as the reptation time [2]. However, some experiments with polydisperse polymers show that this time is much larger than the reptation time, but also shear rate dependent [1]. In this work, we try to elucidate the origin of the repeat shear experiment and exploit its use as a sensitive tool to characterize more complex viscoelastic materials. To this end, we use a supramolecular polymer, which is well-characterized with 2 relaxation times and polydispersity of about 2, akin to wormlike surfactant micelles. Its stress relaxation is a single exponential decay and independent of the average tube length (at different concentrations). We find that the recovery time for the stress peak as measured from the repeated startup experiment, is independent of shear rate and similar to the stress relaxation time measured in the linear viscoelastic regime, likely reflecting the role of break/reformation kinetics in these systems.

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Thursday 15:40 Virtual / Track 11 NF12

Phase transitions of cellulose nanocrystal suspensions via rheo-SIPLI and nonlinear oscillatory shear techniques

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Cellulose nanocrystals (CNC) extracted from the abundant, renewable natural polymer cellulose, show significant potential for many applications, either as material on its own or as renewable reinforcement in polymers. The intrinsic interaction between cellulose nanocrystals results in hierarchical ordering in CNC suspensions. Cellulose nanocrystals (CNCs) can self-assemble into nematic and chiral nematic structures, exhibiting birefringence above a critical concentration. In this work, we explore CNC phases through a combination of rheo-SIPLI (shear induced polarized light imaging) and nonlinear oscillatory shear (Fourier-Transform Rheology and stress decomposition). Aqueous CNC dispersions with concentrations spanning the biphasic (BP) and liquid crystalline (LC) phases (2-9 wt% CNC), as identified based on birefringence, steady shear and linear viscoelastic oscillatory shear data, were investigated. From a nonlinear rheological point of view, for the lowest concentration that approaches the concentrated isotropic - BP transition, a significant angular frequency dependence on the third relative higher harmonic (I3/1) in terms of both scaling exponents, including non-quadratic scaling, and magnitude was recorded. At the transition to LC, I3/1 suggests multiple scaling laws in the MAOS region, including a quadratic scaling strain amplitude range. All concentrations exhibit nonlinear intra-cycle strain stiffening behavior, with weak angular frequency dependence. Already for BP concentrations, a transition from intra-cycle shear thickening to intracycle shear thinning was recorded. The intra-cycle shear thickening behavior was significantly increased for CNC concentrations in the LC phase.

Thursday 16:00 Virtual / Track 11 NF13

Time dependence and hierarchy in cellulose nanocrystal suspensions

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The rheology of high aspect ratio particle suspensions, such as cellulose nanocrystals (CNC), depends to a great extent on the size distribution, the orientation, and the morphology of the rods under shear flow. The CNC suspensions additionally experience a time-dependent flow characteristic, thixotropy. Here, we elucidate time-dependent properties of CNC suspension in 4-8 wt% CNC concentration by four tests that support thixotropy quantification: creep test, complex viscosity, hysteresis flow curve, thixotropy recovery. CNC suspensions exhibit aging and rejuvenation in varying imposed shear stresses in time, and viscosity bifurcation is observed when the viscosity is plotted as a function of time. Combining rheological thixotropy with macroscopic polarized light optical visualization of micro-phase transitions provides a completely new aspect in designing structure of materials from CNC flow. On the other hand, we have also done numerical modeling to predict the time dependency of cellulose nanocrystal. In this model, evaluation of structure parameter is investigated as a function of flow history and shear rate. The model is based on the competition of the system to return to its equilibrium state (restructuring) and its continuous breakage due to flow (destructuring).

Poster Session

Symposium PO

Poster Session

Tuesday 16:00 Virtual / Poster Session 1 PO1

Determination of the molecular weight distribution of ultra-high molecular weight polyethylene from solution rheology

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The rheological determination of material properties (molecular weight distribution, degree of branching, etc) is not always easy to pursue. In particular, when dealing with Ultra-High Molecular Weight (UHMW) polymers, the rheological measurements can be affected by experimental limitations (shear fracture, torque overload, temperature investigation range, loading problems). Diluting the polymer melt into an appropriate solvent [1] may overcome, or at least limit, these experimental issues. In this perspective, rheology can be used as a tool to relate the macroscopic viscoelastic response of polymer systems to their molecular architecture. The aim of this work is to determine the Molecular Weight Distribution (MWD) of a UHMW Polyethylene (UHMWPE) by extrapolating it from the linear viscoelastic response of UHMWPE solutions in a suitable solvent, namely, Low Molecular Weight Polyethylene (LMWPE). The analysis of rheological results is performed by using the time-dependent diffusion/double reptation model introduced by van Ruymbeke [2-3]. This model allows to determine the molecular wight distribution of the melt starting from the linear rheological behaviour of the solution. The MWD results of the model are compared from those obtained independently on the UHMWPE melt.

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Tuesday 16:00 Virtual / Poster Session 1 PO2

Modeling the time and spatial characteristics of flow instabilities for SBR samples during extrusion flow

Christos K. Georgantopoulos[1], Masood K. Esfahani[1], Ingo Naue[1], Andrea Causa[2], Roland Kádár[3], and Manfred Wilhelm[1]
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The flow instabilities [1] for three commercial styrene-butadiene rubbers (SBR) are investigated as a function of molecular weight distribution (MWD) and molecular architecture (linear, branched). Two of the studied samples have bimodal and one unimodal MWD. Deviation from the Cox-Merz rule at high angular frequencies/shear rates become intensive as the amount of low molecular weight (MW) component increased. Optical analysis is used to identify and quantify the spatial characteristics (wavelength and height) of the flow instabilities. Qualitative models [2,3] are used to fit the experimental data for the spatial characteristics of flow instabilities and correlate them with the molecular properties of the samples. Moreover, it is found that the characteristic spatial wavelength increased as the extrusion temperature decreased. Hence, the temperature influence on the spatial wavelength is presented.

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Tuesday 16:00 Virtual / Poster Session 1 PO3

Controlling rheology of a solid emulsion with liquid droplets

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Emulsions are interesting systems whose rheological properties depend on the continuous and dispersed phases and the interface between them. By solidifying the continuous phase and keeping the dispersed phase liquid we can create a composite viscoelastic material that can be tuned by changing the viscosity of the dispersed phase, the elasticity of the continuous phase and/or the surface properties. [1, 2, 3]

We study such a "solid emulsion" with a crosslinked PDMS (poly(dimethyl) siloxane) continuous phase. The dispersed phase is at first pure PEG (poly(ethylene) glycol), or PEO (poly(ethylene) oxide) solutions in PEG in order to vary the viscosity of the liquid phase while keeping it in a

Newtonian regime. Previous theoretical work has shown that we can expect to see different rheological responses depending on the dispersed phase viscosity, the size of the droplets in the solid matrix and the volume fraction of liquid. [1]

The aim of this work is to show the feasibility of a composite system whose storage and loss moduli can be controlled independently, as opposed to the commonly used viscoelastic materials such as adhesives and gels.

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Tuesday 16:00 Virtual / Poster Session 1 PO4

Preliminary rheological testing of smart hydrogels formulated with hybrid carrageenans applied to 3D printing

M.D. Torres, M. Álvarez-Viñas, V. Sanz, N. Flórez-Fernández, and H. Domínguez
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In recent years, natural polymers from marine-derived resources have gained growing attention for emerging technologies as 3D printing [1]. Further development of the new 3D biopolymer-matrices field lies in smart materials with satisfied printability, mechanical integrity, and biocompatibility. Hybrid carrageenans could be atractive alternatives with potential for several applications because of their suitable chemical structures or mechanical functionalities [2]. In this context, the main aim of this work was the rheological study of a number of hybrid carrageenans extracted using eco-friendly treatments in order to assess its feasibility for 3D printing. For this end, C. crispus and M. stellatus red seaweeds from the Galician coast were used as raw materials. The corresponding hybrid carrageenans were extracted using optimized procedures of autohydrolysis by conventional or microwave heating. Rheological performance of the hydrogels applied to 3D printing formulated with above biopolymers was evaluated by both steady-state and dynamic oscillatory shear measurements. 3D printing parameters (e.g. noodle size, print speed, flow temperature or line thickness) were tailored based on the rheological testing. Selecting the 3D printing variables properly, both autohydrolysis by conventional and microwave heating were able to provide hybrid carrageenans with adequate mechanical features in order to achieve printable hydrogels. Note here that the lowest noodle sizes (< 1.5 mm) with low printing speeds (<1500 mm/min) resulted in better printability. Overall, it should be highlighted the social value of the rheological testing, which is crucial in the context of 3D printing, by validating its relevance on the characterisation of the performance of sustainable biopolymers for industrial and everyday life applications.

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Tuesday 16:00 Virtual / Poster Session 1 PO5

Rheological behavior of shear-thickening nanofluids: effect of combination and pre-shear

Parvin Alaee, Milad Kamkar, and Mohammad Arjmand
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In this work, the shear thickening behavior of silica 816 (slightly hydrophobic) and silica 200 (hydrophilic) nanoparticles (NPs) in polyethylene glycol (PEG) was investigated using rheological characterization in steady state flow mode. Afterward, hybrid suspensions of silica 200-silica 816 NPs/PEG were prepared. The viscosity curve of the hybrid samples was compared with silica 200/PEG and silica 816/PEG. The results showed that incorporation of two different nano silica particles into the nanofluids increased both critical shear rate (i.e., onset of shear thickening behavior) and extent of shear thickening compared to that of the single nanofluids. The effect of pre-shearing on viscosity behavior of silica/PEG samples was also studied. To achieve this, samples were pre-sheared at three different shear rates (i.e., 10, 20, 30 s^{-1}). The result showed that pre-shearing changed the shear rate dependency of the viscosity for both silica 200/PEG and silica 816/PEG, however, silica 816/PEG showed no sensitivity to the applied pre-shear value. For silica 200/PEG, the extent of shear rate and critical shear rate decreased by increasing pre-shear value.

Tuesday 16:00 Virtual / Poster Session 1 PO6

Linear viscoelasticity of polyethylene oxide nanocomposites

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Composites of high molecular weight polyethylene oxide(PEO) and silica nanoparticles show a unique shear-thickening behavior. While the non-linear viscoelasticity of such composites has been widely studied, there are few systematic studies on their linear viscoelasticity, which is important to understand the thermal equilibrium dynamics of polymers and particles. In this study, we aimed to elucidate the relation between the macroscopic properties and microscopic dynamics of PEO/silica composites by systematically measuring the linear viscoelasticity with varied PEO molecular weight and silica concentration.
The linear viscoelasticity was measured by creep tests and frequency sweep tests. The molecular weight of PEO was 4.0×10^5 - 1.0×10^6 (g/mol) and the concentration of silica was 5.3 - 11 (vol%).
The addition of nanoparticles led to more than a tenfold increase in the relaxation time and complex modulus compared to a pure PEO solution. Such an enhancement in viscoelasticity could not be explained by the stress and strain amplification of the polymer matrix caused by the particles. To clarify the microscopic dynamics underlying the viscoelastic enhancement, we defined an "additional term" by subtracting the contribution of

the polymer matrix from the overall complex modulus of the composite. The PEO molecular weight and silica concentration dependencies of the additional term were consistent with that of an ideal suspension (i.e. a suspension with a predominantly repulsive particle interaction.) On the other hand, the absolute value of the composite's relaxation time was more than 100 times longer than the predicted relaxation time of an ideal suspension.

These results suggest that the viscoelasticity of PEO/silica composites mainly originates from the diffusion of nanoparticles, and that the nanoparticle diffusion is delayed by the high viscosity of the polymer matrix and the attractive interaction between PEO and silica.

Tuesday 16:00 Virtual / Poster Session 1 PO7

Rheological evaluation of the preparation of microfluidized pea fibre suspensions

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Functional and structural properties of fibres can be improved by mechanical processing. Rotor-stator homogenizers can reach shear rates like those generated by colloid mills and lower than high-pressure valve homogenizers and microfluidizers. Microfluidizers are the devices that generate the highest shear rates among all commercial homogenizers. This contribution deals with a comparative study of the linear dynamic viscoelasticity (SAOS) of pea outer fibre suspensions prepared by different methods based on microfluidization, using two Z-shaped shearing cameras in series. In all cases, the microfluidizer was fed by a primary suspension previously prepared by a semi-batch toothed rotor-stator homogenization process followed by a batchwise step. We show that 1 pass through a microfluidizer at high pressure led to poor reproducibility and syneresis as demonstrated by monitoring multiple light scattering data. This problem could be overcome by further mixing with a sawtooth-type impeller or by submitting the primary suspension to 3 passes through the microfluidizer. In both cases a flat dependence of the loss tangent (values around 0.1) with frequency was observed, congruently with the occurrence of anisotropic gel-like domains as demonstrated by polarized light microscopy. Interestingly, the highest G' and G" values were obtained by the sample prepared by microfluidization after 3 passes. This technique turned out to be more successful to promote defibrillation and interactions among cellulosic strands due to the increase in surface area achieved thanks to the thanks to the combination of high shear and extensional deformation in the microfluidizer microchannels. The conclusions drawn from this study point to the need to optimise both the fiber concentration and microfluidization pressure to obtain a more homogeneous microstructure.

Tuesday 16:00 Virtual / Poster Session 1 PO8

miTT – a new measurement protocol to obtain rich rheological data for emulgels and other heterogeneous systems

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Disperse systems, such as blends, emulsions, colloids, and composites, tend to adjust their structure depending on the deformation history and, thus, are more difficult to characterize than single phase materials. Thixotropy is typically found in disperse systems and classically characterized with a thixotropic loop test. In the last years, the 3iTT protocol - a dynamic-mechanical test (DMT) at low deformation and constant frequency, followed by a start-up flow (SUF) at constant shear-rate, and then the same DMT - was developed as an alternative to check for changes in material behavior due to defined shear deformation. Based on this, we developed the multiple interval thixotropic test protocol (miTT), where the same DMT is conducted after an SUF under variation of the constant shear rate (0.1, 0.3, 1, 3, 10, 30, 100, 300, 1000, 300, 100, 30, 10, 3, 1, 0.3, 0.1 1/s). The results of this test routine are a viscosity function η(shear rate) with increasing and decreasing shear rate and G' (shear rate of previous test) and G" (shear rate of previous test).

We tested the setup on oil in water graphene oxide Pickering emulsions and several other conventional emulsions. The viscosity function determined from this experiment matched the viscosity functions determined through regular experiments with high accuracy. More importantly, the G' and G" are strongly influenced by the previously applied shear rate. While regular emulsions show a decrease of G' and G" upon a higher shear rate in the previous shear step, the Pickering emulsions show an increase. In both cases the change is approximately reversible, i.e. G' and G" depend on the shear rate in the previous shear step and not on the complete previous shear history. The changes in G' and G" correlate well with the emulgel composition, especially with the Pickering emulsifier content.

Tuesday 16:00 Virtual / Poster Session 1 PO9

Changes of blood rheological properties and biochemical markers after participation in XTERRA Poland triathlon competition

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The importance of physical activity in preventing chronic cardiovascular and metabolic diseases and the role of exercise as an adjunct therapy is widely recognised. However, prolonged and intensive exercise is known to cause changes in blood rheological properties and biochemical markers, and sometimes athletes participating in strenuous competitions need medical attention. To understand the phenomena occurring in the body in such situations, we decided to study the biomarkers after XTERRA Poland 2017 triathlon competition. Blood samples were collected 24 hours before, immediately after, and 16 hours after the competition (n = 10). Immediately after the race, the white blood cells count (WBC), platelets, uric acid and interleukin-6(IL6) levels were significantly ($p< 0.001$) increased, and hematocrit (HCT), Na^+, Cl^-, IgA were decreased. The following day there were clinically significant changes in Na^+, Cl^-, CRP levels were significantly ($p< 0.001$) increased, and the white blood cells count (WBC), the red blood cells count (RBC), haemoglobin (HGB), hematocrit (HCT) , MCV, platelets, IgG, IgA, IL-6 were decreased.Analysis of the remaining rheological indices did not show any statistically significant changes. In conclusion, assessing rheological parameters such as erythrocyte deformability and aggregation, is useful for monitoring the adverse effects of intensive and exhaustive exercise.

Tuesday 16:00 Virtual / Poster Session 1 PO10

Evaluation of the rheological-thermal behaviour of protein-based systems with incorporated salts

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Proteins are biopolymeric systems that can be formed as bioplastics through the application of temperature and/or pressure. In this way, protein-based systems can be processed by thermomoulding techniques such as injection moulding, extrusion or thermocompression. Usually, a plasticizer is added to these proteins to improve the chain mobility and to reduce the transition temperature of these systems during their processing. Furthermore, some additives, such as salts, can be incorporated to modify some of the bioplastic properties. However, these additives can also vary the thermal profile of the systems and, thus, changing the optimal conditions for their processing. In this sense, the main objective of this work was to evaluate the thermal profile of soy protein-based systems and their modification when different salts (zinc sulphate monohydrate and zinc-EDTA) are incorporated in these systems. In order to evaluate these profiles, rheological temperature tests were carried out. In addition, the thermal information provided for these tests was contrasted with differential scanning calorimetry and thermogravimetric analyses, to assess the validity of rheological studies to obtain the thermal behaviour of protein-based systems. The results showed that the inclusion of plasticizer notably reduces the glass transition temperature of the protein, allowing its aggregation at a certain temperature. On the other hand, the salt incorporation generates changes in the aggregation point, which is dependent on the salt structure, improving or worsening the bioplastic processing. Finally, rheological temperature tests have managed to provide information of great interest in the processing of these systems, similar to the information obtained by more specific tests.

Tuesday 16:00 Virtual / Poster Session 1 PO11

An edible humidity sensor

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We report an edible humidity sensor made up of a protein, caseinate, and a molecular vitrifier, glycerol, that mechanically bends upon exposure to humidity. The sensor is a composite material made up of two interfused protein films with varying caseinate and glycerol concentrations. Upon exposure to humidity, two interfused films absorb different amounts of water and bend to report on humidity. To rationally engineer the sensor for maximum bending, we characterized the vitrified protein films with rheology as well as gravimetric analysis and propose a mechanism relating the microstructure to mechanical response. Moreover, we demonstrate that the degree of bending can be tuned by sensor geometry, layer thickness and caseinate/glycerol ratio. Currently, we are exploring 3D printing techniques to better control the humidity response and extend the applicability of the proposed sensor. We hope that the proposed edible sensor can be placed inside perishable food and pharmaceutical products directly reporting on humidity where it matters, a feat commercial non-edible electronic and chemo-chromatic sensors cannot provide.

Tuesday 16:00 Virtual / Poster Session 1 PO12

Rheology and texture analysis of fun foods

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The global demand for foods is huge! Myriad types are produced to suit a broad spectrum of tastes. Prepackaged, processed foods are very convenient to millions of consumers. Rheological and Texture Analyses provide quantitative values that are used in process equipment design and correlate to consumer acceptance. Different test protocols provide data ranging from R&D to QC/QA applications. This presentation illustrates different measurement techniques and discusses data for some common foods.

Tuesday 16:00 Virtual / Poster Session 1 PO13

Tracking of red blood cells in a comoving frame during microfluidic flows

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One of the most intriguing features of red blood cells (RBCs) is their high deformability that allows them to squeeze through microvessels smaller than the RBC size. Additionally, this flexibility results in a broad range of RBC shapes in microfluidic flows, depending on their confinement and flow velocity. To study their flow and shapes in microfluidic devices, RBCs are often recorded at a fixed channel position using optical microscopy. However, this approach limits investigations of the RBC flow behavior and shape transitions to merely a few hundred micrometers, depending on the used camera and objective. In this study, we present a microfluidic technique that allows us to track RBCs over several

centimeters along the channel flow direction. The microfluidic setup consists of an inverted microscope, equipped with a motorized stage, a 20x objective, a highspeed camera, and a high-precision pressure device to generate a time-dependent driving of the flow. We use a customized feedback-control mechanism between the stage and camera to obtain a comoving frame. RBCs are instantaneously tracked and the observation frame follows the cells in the microfluidic device with a velocity of up to 10 mm/s. Our method enables us to probe the flow behavior and shape transitions of individual RBCs along the whole channel length both under steady and pulsatile flow. Thus, the presented technique opens new pathways to study cell dynamics and interactions in microfluidic devices under physiologically relevant flow conditions.

Tuesday 16:00 Virtual / Poster Session 1 PO14

Nonlinear viscoelastic rheology of wheat dough examined through classical constitutive equations

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With the emergence of large amplitude oscillatory shear (LAOS) as a powerful tool to characterize the viscoelastic behavior of materials, it is evident that LAOS is even more appropriate to study the rheology of food materials as they exhibit nonlinear behavior at exceedingly small deformation. In this work, the power model is used to describe the linear behavior of dough. The Johnson-Segalman model, the Giesekus model and the Phan-Thien Tanner models are not able to describe the the strain softening behavior of bread dough due to the limits on the numerical values of the respective models' nonlinear parameters. The Larson model, K-BKZ model and the Lodge-damage models exhibit strain softening, but the K-BKZ model and the Lodge-damage model provide a better description of bread dough strain softening than the Larson model. The Larson model, the K-BKZ model and Lodge-damage model are examined at large amplitude oscillatory shear (LAOS) conditions. At LAOS conditions, it is found that the Lodge-damage model displays unrealistic Lissajous stress-strain plots.

Tuesday 16:00 Virtual / Poster Session 1 PO15

Enhancing the nanomechanical properties of CNC/PEG composite films by the application of shear field

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Self-assembly behavior of cellulose nanocrystals (CNCs) into liquid crystalline (LC) structures is of growing interest in the recent years due to its potential for generating biocompatible, biodegradable smart materials with unique mechanical and optical properties. The applicability of CNC films can be improved by incorporating CNCs into a nonadsorbing polymer matrix such as polyethylene glycol (PEG). The properties of the LC assemblies by CNC particles can be manipulated by the application of shear force, electrical or magnetic field, and by varying the environmental conditions such as temperature, humidity etc. Hence, the mechanical and optical properties of the composite films can be fine-tuned. In this work, we investigate the effect of shear flow in the assembly of the CNC particles in the CNC/PEG nanocomposite films at various CNC:PEG ratios. Rheology, polarized optical microscopy (POM) and nanoindentation are employed to explore the link between microstructural evolution during flow and mechanical performance of the composite films. The rheology of CNC/PEG dispersions in water showed increasingly shear thinning behavior with increase in PEG concentration. The nanomechanical studies evidently showed a significant improvement in the reduced Young's modulus and hardness of the shear-dried films, in comparison with the non-sheared films, due to the improved orientation of CNC particles owing to the shear flow. Moreover, this effect is observed to be predominant at higher concentrations of CNC (75-100%). POM observations showed the formation of cholesteric LC with characteristic finger-print textures due to the helical orientation of CNC particles, at high CNC concentrations. Whereas, increase in concentration of PEG leads to the crystallization and formation of PEG spherulites with microscopic scale phase separation. This is manifested as a monotonous decrease in the reduced Young's modulus and hardness of the composite film as the concentration of PEG varied from 0% to 100%.

Tuesday 16:00 Virtual / Poster Session 1 PO16

Coupling of shear rheology with time- and space-resolved dynamic light scattering - role of normal stress in the creep dynamics and failure of a biopolymer gel

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Material failure is widespread and occurs on vastly different length scales, from earthquakes to the atomic level. It often involves sudden and unpredictable events, with little or no macroscopically detectable precursors. A better understanding of the mechanisms leading to failure is however highly desirable and would have deep implications, possibly paving the way to predicting failure. We will present experiments that probe the delayed rupture of biopolymer gels under a constant shear load, using an original set-up that simultaneously probe the macroscopic rheological response and the microscopic structure and dynamics of a gel submitted to a constant shear stress [1, 2]. We unveil the crucial role of normal stresses built up during gelation: all samples that eventually fracture self-weaken during the gelation process, as revealed by a partial relaxation of the normal stress concomitant to a burst of microscopic plastic rearrangements. Upon applying a shear stress, weakened gels exhibit in the creep regime distinctive signatures in their microscopic dynamics, which anticipate macroscopic fracture by up to thousands of seconds. The dynamics in fracturing gels are faster than those of non-fracturing gels and exhibit large spatio-temporal fluctuations. A spatially localized region with significant plasticity eventually nucleates, expands progressively, and finally invades the whole sample triggering macroscopic failure.

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[2] Pommella, Cipelletti, Ramos. Role of normal stress in the creep dynamics and failure of a biopolymer gel. PRL 125, 268006 (2020)

Tuesday 16:00 Virtual / Poster Session 1 PO17

Effect of operating parameters on the rheological properties of licorice extract

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Licorice extract is a product, used in different areas of food industry, obtained from the root of licorice (Glycyrrhiza glabra), a plant of the Leguminosae family native to Southern Europe and Asia. The extraction process is performed mixing hot water, as solvent, and grinded licorice root; the diluted solution obtained after this extraction step is then concentrated up to the desired value (depending also on the final use). High temperature is used during both extraction and concentration aiming at improving the extraction yield and the final productivity because it increases thermodynamic solubility limits of some components and mass transfer rate. Nevertheless high temperatures cause thermal degradation (such as Maillard reaction) of some components (such as polysaccharides) modifying the rheological properties of the final product. A good knowledge of the rheological behavior of extract is necessary in quality control and in engineering applications involved in the proper design and management of unit operations. In this work licorice extracts were produced using a lab-scale system where extraction and concentration were carried out. In order to minimize the potential effects of raw material variability, experimental tests were performed using licorice roots from a single lot. Extraction was performed at 120 °C for 210 min using water to licorice root mass ratio of 5:1. The concentration was performed by changing operating conditions (100°C-1 bar; 80°C-0.5 bar; 60°C-0.2 bar) with the aim of investigating their effects on rheological characteristics of final products having different concentrations (21-30-40 °Brix). Obtained results revealed that viscosity and dynamics modulus (G' and G") increase with extract concentration and decrease with decreasing the adopted process temperature.

Tuesday 16:00 Virtual / Poster Session 1 PO18

Computation of transient Bingham-Carreau-Yasuda pipe flows

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A coating process is generally designed based on the behaviors of the steady-state flows. However, in industrial applications, there are many external disturbances in the process, such as flow rate oscillations from flow pumps. When such disturbances are transmitted to flows, the performance of the final product may be significantly impaired due to deleterious effects. A yield behavior is observed in many structured fluids such as slurries, pastes, or polymer solutions, and such fluids exhibit different flow characteristics from traditional Newtonian fluids. Therefore, we specifically focus on transferring complex fluids through pipe systems when flow disturbances are present.

In this study, Bingham-Carreau-Yasuda (B-C-Y) model, which has an extra term representing yield behavior in addition to the well-known Carreau-Yasuda model, is used to model complex fluid. The solution is computed with the method-of-lines approach using the finite element method (FEM) and the trapezoid rule (TR) with finite difference interrupts (FDI). The validity of the implemented numerical scheme is tested with known analytic solutions. Then, transient responses of B-C-Y pipe flows with various frequencies are analyzed, and the results are compared with Newtonian pipe flows.

Tuesday 16:00 Virtual / Poster Session 1 PO19

The thixo-elastoviscoplastic behavior of blood in pulsatile flows

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This work presents an in silico investigation of the pulsatile blood flow in straight, rigid tubes and a 3D carotid geometry extracted by MRI. We invoke an advanced constitutive modeling for blood rheology based on a thixotropic-elasto-viscoplastic formulation (TEVP), which is fitted on steady, simple shear, and transient multi-shear-rate experiments, providing a very good agreement. This model accounts implicitly for the aggregation occur in low shear rates through a microstructural kinetics equation, which describes the level of blood structure at any instance. The investigation is implemented for both sinusoidal and real pressure-gradient waveforms with different frequencies, amplitudes, and patterns. A significant contribution of the normal stress to the total stress tensor is addressed while the phase lag between the pressure-gradient and the flow-rate increases with both frequency and amplitude. The impact of the Womersley (Wo) number on the flow field is high, yielding complicated velocity profiles and shear/normal distributions within the tube. We also provide a detailed prediction of the hemodynamics under various real waveforms regarding the normality/abnormality, reversal of the flow, and the magnitude of the waveform amplitude. To describe the unsteady nature of blood flow, we calculate the oscillatory shear (OSI) and normal (ONI) indices while the phase lag varies between 10 to 40 of degrees. Our investigation is enhanced by a 3D simulation of the blood flow in a carotid bifurcation, the local hemodynamics of which is associated with the onset and progression of vascular diseases. We also address the impact of the real pulse waveform on both shear and normal stresses distribution, especially near the artery bifurcation, where the aggregation is intense as a consequence of low stresses.

Tuesday 16:00 Virtual / Poster Session 1 PO20

Physico-mechanical characterization of polyurethanes for cosmetic use: rheology and texture analysis

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Product innovation is a crucial factor in a continually growing competitive market. Cosmetic industries are seeking new raw materials to create formulas that could satisfy consumers' expectations of efficacy and sensoriality. Nowadays, innovation also involves sustainability, as the attention on the environmental impact is increasing. Recently, the chemistry of polyurethanes has aroused considerable interest, because of their versatility, the ability to create engaging textures, and their possible biodegradability. The aim of this work is to characterize the physical-mechanical properties of two polyurethane-based raw materials, used alone or in associations, evaluating their ability to stabilize and thicken cosmetic hydrogels and emulsions: X (Polyurethane-59, Butylene glycol, Aqua, Tocopherol) and Y (PEG-240/HDI copolymer BIS-decyltetradeceth-20 ether, Butylene glycol, Water, Potassium laurate, Tocopherol). The rheological analyses were conducted both in continuous and oscillatory flow conditions using a rotational rheometer, with a plate-plate geometry at a fixed gap of 1 mm. The systems' texture properties were analyzed through an immersion/de-immersion test by means of a Texture Analyzer, equipped with a spherical probe. According to the different chemistry of the polyurethanes, the data pointed out two different profiles: X showed a weak-gel pattern of G' and G" in function of the frequency and higher values of firmness and consistency, while Y showed viscoelastic properties with high adhesiveness and a stringy behaviour. Therefore, the binary associations of these two raw materials combined in appropriate ratios allowed modulating the spreading and the pick-up properties, obtaining a wide range of different textures. This study demonstrates that the combined use of rheology and texture analysis, which are significantly correlated, represents a valid protocol to study semi-solid systems, rationalize the use of polymers enhancing the sensory profile of cosmetic products.

Tuesday 16:00 Virtual / Poster Session 1 PO21

Rheology and mesophase separation transition in olefin block copolymers

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The structure of olefin block copolymers consists of a statistical sequence of hard and soft blocks. The hard blocks are rich in polyethylene whereas the soft blocks are rich in a longer a-olefin comonomer, generally octene. Above the melting temperature of the hard blocks, such systems can be easily processed as thermoplastic materials. However, upon cooling, the hard blocks undergo crystallization while the soft blocks are still above their glass transition. In this state, olefin block copolymers display excellent elastomeric properties and, as such, they are used in a broad range of applications. Recent advances in synthetic chemistry allowed for an economically favourable one-pot synthesis of olefin block copolymers through a chain shuttling polymerization process. By varying the reaction parameters, in example the ratio of polyethylene to a-olefin, it is possible to tune, to some extent, the total molecular weight, the total comonomer content, the relative length of the blocks and the difference in comonomer content between the hard and the soft phase. The parameters above influence both mechanical and rheological properties. In particular, the total comonomer content affects the crossover time and the crossover modulus. The difference of a-olefin content between the hard and soft blocks is relevant for the crystallization properties and the structure fluctuations above the melting temperature. Molten olefin block copolymers undergo a mesophase separation transition whose extent increases with increasing comonomer content and lower temperature. In this study we present a systematic study of the rheology and the order-disorder fluctuation properties of olefin block copolymers depending on the type of comonomer and the difference in comonomer content between the hard and soft blocks. A method for a quantitative analysis of the mesophase separation is also proposed.

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[2] Park et al. Macromolecules 43 (2010), 6789;
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Tuesday 16:00 Virtual / Poster Session 1 PO22

Novel non-aqueous stearic acid-in-silicone oil (o/o) phase change emulsion as thermal energy storage and transport media

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Phase change emulsion (PCE) is a kind of two-phase heat transfer fluid with phase change material (PCM) dispersed in a carrier fluid. It has received intensive attractions in recent years since it can be used as both the thermal energy storage material and transport medium simultaneously in a thermal energy storage system. The present work was aimed at formulating stable non-aqueous emulsions of stearic acid with a melting peak temperature of 68-71ºC and silicone oil in order to explore using such systems as novel phase change material (PCM) emulsion. Little work has been done in incorporating PCMs in water with the help of emulsifiers and, to the best of our knowledge, there are almost no reports studying non-aqueous emulsions with such application. Manufacture of these emulsions has been a complicated task due to the major difficulty in formulating stable non-aqueous emulsions, arising from the lack of data regarding the availability of suitable surfactants in such systems. Thus, anhydrous stearic acid-in-silicone oil emulsions stabilised with a selected silicone surfactant containing diblock copolymers along with bulky silicone chains were prepared in this study. The morphology, thermophysical properties, rheological behaviour and viscoelasticity of the emulsions were measured and analysed. According to the results, the properties of the emulsion were greatly influenced not only by the amount of dispersed phase present in it but also by the speed of crystallization of this phase. Moreover, the present PCE were able to resist heating-cooling cycles and remain stable at ambient temperature for at least one month, keeping its heat storage capacity intact. Therefore, resultant emulsions are very promising materials not only for its potential use in cosmetic and pharmaceutical applications thanks to its oily composition but also for heat storage technologies.

Tuesday 16:00 Virtual / Poster Session 1 PO23

A comparative study of the effect of microfluidization and rotor-stator mixing for producing dietary fibre suspensions

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Dietary fibre is an important supplement to improve consumers' health; many studies confirm that high dietary fibre consumption reduces the risk associated with many chronic diseases. In addition, from a technological point of view, dietary fibre can produce "gel-like" materials when added to an aqueous phase; in fact, fibre can bind water and produce a network able to entrap the solvent. Different processes can be used for dispersing fibre in water, thus affecting the final properties of the derived suspensions. This work aims at investigating the effects of different devices on the rheological properties and microstructure of fibre suspensions added to water at a fixed concentration. In particular, a rotor-stator mixer and a high-pressure homogenization via microfluidization process were used; these devices are able to generate different maximum shear rates allowing the study of distinct process conditions to be investigated. At first, a preliminary study of the effects of rotor-stator homogenization on the rheological and microscopic properties of suspensions was carried out. It was observed that the trend of dynamic moduli evaluated with Small Amplitude Oscillation Tests are affected by the power of mixing that, in turn, does not influence the particles size distribution of the system. Samples prepared with the same formulation, were, therefore, mixed at two operating pressure (corresponding to two different power values) with the Microfluidizer; the characteristics of samples prepared with both techniques were compared, evidencing some differences in structuration degree, Sauter diameter and microstructure, whereas no significant differences between the strength of the network was observed.

Tuesday 16:00 Virtual / Poster Session 1 PO24

Investigation of the rheological properties of a novel natural surfactant–polymer system for enhanced oil recovery application

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Surfactant has a significant role in enhanced oil recovery (EOR) as it can notably reduce interfacial tension and modify the wettability between oil and water in the reservoir. Mostly synthetic surfactants are highly being practiced in EOR. However, these surfactants harm the environment attributable to their toxic and non-biodegradable nature. This work is focused on the performance assessment of a natural surfactant derived from Eichhornia crassipes weed and its utilization in EOR. The influence of the synthesized natural surfactant on the rheological properties of conventionally used polymers (i.e., xanthan gum and polyacrylamide) has been studied and compared with that of a commercially used surfactant (i.e., sodium dodecyl sulfate). Effective improvement in the rheological properties and stability against reservoir-like conditions suggests the potential application of synthesized natural surfactant in EOR.

Keywords: Enhanced oil recovery, interfacial tension, natural surfactant, polymer, rheology

Tuesday 16:00 Virtual / Poster Session 1 PO25

RepTate rheology software for the analysis of theories and experimental data

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In this poster, we present the free and open source RepTate (Rheology of Entangled Polymers: Toolkit for Analysis of Theory and Experiment) software package for viewing, exchanging and analyzing rheological and associated data. RepTate provides a powerful and user-friendly platform that simplifies the comparison of experimental data with theories very easy. The software can be run on Windows, Mac and Linux, and can be installed in the same computer that controls the rheometer. Here, we showcase some of the common uses of RepTate by reproducing predictions of recently published articles, from entangled, mono- and polydisperse, linear chains to branch-on-branch polymer systems, in the linear and nonlinear rheology regimes.

Tuesday 16:00 Virtual / Poster Session 1 PO26

Impact of olive oil by-products extracts in the rheology of topical creams

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Olive oil by-products present a great interest in the pharmaceutical, cosmetic and food industries, mainly due to their several bioactivities and health promoting properties, such as antioxidant, anti-inflammatory and photoprotector. Their application has also been studied in cosmetic and in dermatology research field for the treatment of skin diseases using different topical delivery systems. Nevertheless, the incorporation of natural ingredients may cause an impact on creams' structure leading to changes in its appearance as well as its physical-chemical and rheological properties. Therefore, the main aim of the present work was to evaluate the impact of three different olive by-products extracts, obtained without using organic solvents, on the rheological characterization in oil-in-water (O/W) creams. Three creams (cream 1, 2 and 3) were prepared using 5% of three different olive oil extracts. Continuous shear techniques ($0.1s^{-1}$ to $100s^{-1}$) and in the viscoelastic region using oscillation techniques (frequency sweep test with a shear strain of 0.1% and a frequency range between 0.1 and 10Hz) were performed using a Kinexus Lab+ Rheometer (Malvern, UK). Comparing the results obtained with the control cream (without extracts) is possible to demonstrate that all extracts influenced the internal structure of the creams. Furthermore, all formulations are classified as shear thinning emulsions, in which can be easily rubbed into the skin. For all creams, the best fitting model is the Herschel-Bulkley model, which presents a correlation coefficient equal to or higher than 0.996 for all formulations. This model describes a material with a non-linear behavior and it identifies the power law index (n). Regarding the results, the power law index varies between 0.410 and 0.559, confirming the shear thinning behavior. Furthermore, the control cream presents the highest yield stress value, namely 1.459 Pa, meaning that this emulsion presents a consistent and a cohesive structure.

Tuesday 16:00 Virtual / Poster Session 1 PO27

Extensional rheology of human blood analogues under the action of magnetic fields

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Blood rheology is highly dependent on plasma viscosity, hematocrit and mechanical properties of red blood cells. Nevertheless, the application of external forces as magnetic fields to blood flow can significantly affect its rheological behaviour. Recent studies showed that the viscosity of blood could be increased significantly by applying a magnetic field to the bloodstream when magnetic particles are added to flow [1]. Therefore, a complete rheological characterization of the blood loaded with magnetic particles under the action of external magnetic fields is of high interest, as it can be the basis for the development of new patient treatments and new biomedical applications.

As a first approximation, rheological human blood analogues were used. An aqueous solution of 52 wt.% of dimethyl sulfoxide (DMSO) was prepared as Newtonian blood analogue. For the viscoelastic blood analogues, a mixture of 100 ppm of Xanthan Gum (XG) in an aqueous solution of 52 wt.% was formulated according to [2]. Another four solutions based on the same XG mixture were prepared with different concentrations: 250, 500, 750 and 1000 ppm as in [3]. Micron-sized magnetic particles were added to the blood analogues solution.

A capillary break up extensional rheometer (CaBER) will be used to assess the longest relaxation time of the blood analogues. For the assessment of the extensional properties, a high-speed camera was used to follow the time evolution of the filament thinning. The external magnetic field was imposed parallel and perpendicular to the extensional flow, as in [4]. Results showed a great influence on the extensional properties of the analogues when the magnetic field is increased. Also, clear differences between the parallel and perpendicular configurations.

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[1] P30.00002 in the 72nd Annual Meeting of the APS DFD 64, 13 (2019).
[2] Biomicrofluidics, 7:034102,(2013).
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Tuesday 16:00 Virtual / Poster Session 1 PO28

Rheology as a predictive tool for selecting the optimal printing parameters in an extrusion-based 3D printing process

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Extrusion-based 3D printing has recently gained popularity in pharmaceutical applications due to the ability of print customized drug delivery systems (DDS). The research project aimed to study the rheological properties of a gelatin-based hydrogel ink to determine the optimal printing temperature and printing speed, using a Quality by Design approach. To meet this goal, rheological measurements were performed using a controlled stress Kinexus Lab+ Rheometer (Netzsch, UK). A single frequency strain controlled with temperature ramp test was performed to determine the gelation time and the optimal gelation temperature (Frequency: 1 Hz; start temp: 60°C; end temp: 25°C). For evaluate the printability, an extrusion-based 3D bioprinter (Allevi 2) was used. The printing fidelity (PF) and geometric accuracy (GA) was analysed by measuring the filament diameter of the printed filaments extruded under different pressures. The viscoelastic data collected indicate that the phase transition occurred between 220-250s ($Tan(\delta)<1$), corresponding to a temperature between 42.4-39.8°C. Suggesting that for increase the PF and PA and reduce the extrusion pressure during printing a temperature > 43°C should be considered. The experimental design revealing that temperature causally affects the viscosity and consequently the filament uniformity and the printing quality. The obtained results revealed that the filament uniformity increase with the decrease in temperature. At low temperatures the filament diameter is more homogeneous, uniform and the spreading ratio is lower compared to high temperatures. A combined evaluation of printability and rheological properties showed that at a low temperature the filament stability after extrusion increases which results in high geometric accuracy and shape fidelity. In conclusion, the application of rheological studies during the optimization of an extrusion-based 3D printing process is essential to increase the knowledge over the viscoelastic behavior of temperature sensitive hydrogel inks.

Wednesday 15:40 Virtual / Poster Session 2 PO31

Effect of carbon nanotube aspect ratio on linear and nonlinear rheology of polymer nanocomposites

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In this work, high-density polyethylene (HDPE) was melt-mixed with various loadings of custom-synthesized multiwalled carbon nanotube (CNT) to create conductive polymer nanocomposites (CPNs). These CPNs can be tailored to obtain an optimum combination of properties for electrical and strain-sensing applications. The custom-made CNTs were synthesized via a novel catalyst preparation technique and varying synthesis times, which provided a unique opportunity to investigate the effect of nanotube aspect ratio on nanofiller network structure (i.e., dispersion quality). In the first step, we studied the linear rheological response of the samples. Subsequently, we scrutinized the correlation between rheological response and electrical properties in the molten state with respect to strain amplitude under small, medium, and large amplitude oscillatory shear flows (SAOS, MAOS and LAOS, respectively) by utilizing state-of-the-art dielectro-rheological spectroscopy. In each regime, we studied the intracycle rheological response of the samples utilizing output stress waveforms and Lissajous-Bowditch plots. Dielectro-rheological results showed that the electrical properties of nanocomposites containing CNTs with higher aspect ratio are strain invariant while their rheological responses are highly sensitive to the strain. On the contrary, nanocomposites with CNTs possessing lower aspect ratio followed an opposite trend, indicating that electrical properties were highly dependent on strain, but rheological behavior had low sensitivity to strain. Analyzing the viscoelastic responses of the nanocomposites with the aid of output stress waveforms and Lissajous-Bowditch plots demonstrated significant differences in microstructural features of the nanocomposites, highlighting the importance of CNT physical structure. Novel aspects of this work will serve as a guide for designing and tailoring smart composite materials and assist in understanding and tuning their strain responses.

Wednesday 15:40 Virtual / Poster Session 2 PO32

From bubbles to "doubles"

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We report the formation and breakup of Newtonian and viscoelastic spherical interfaces surrounded on both sides by a Newtonian immiscible liquid. The interface is created with a capillary tube which is submerged in a viscous Newtonian oil by pinning a droplet of another immiscible liquid at the tip of the tube. The external phase is then pumped through the capillary tube at which point an interface starts developing. In this way, the interface is surrounded on both sides by the more viscous phase. We call these spherical interfaces "doubles" by analogy with soap bubbles where the external gaseous phase is replaced by an immiscible liquid. As the spherical "double" grows, it will eventually reach a critical thickness which prohibits any subsequent growth. The breakup process will then lead to the formation of filaments which ultimately transform into droplets via Rayleigh-Plateau instability. Special attention is given to the fluid structures generated by the breakup process and the growth of the spherical interface.

Wednesday 15:40 Virtual / Poster Session 2 PO33

Bubble rise in a viscoelastic fluid

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Bubbly liquids are dispersions of bubbles in liquids. They are metastable. Liquid drains between the bubbles under gravity and the liquid sepaterates into two phases. Bubbly liquids exist commonly in nature and play a significant role in energy-conversion, oil and chemical industries.Therefore understanding how bubbles rise and liquid drains is of great importance. The problem has been investigated in earlier studies for single bubbles and bubbles clusters rising in Newtonian fluids and viscoelastic fluids [1]. In our work, we extended these studies to much larger gas fractions (up to 30%, while in the earlier studies the gas fraction was below 10%). We report on the bubble rise velocity in micellar solutions made of cetyltrimethylammonium bromide (CTAB) and sodium salicylate (NaSal). When the NaSal concentration is increased, the micelles elongate and become wormlike. The viscosity increases and the solutions become shear-thinning with a yield stress. In the Newtonian fluids the bubble rise velocity decreases with increasing volume fraction of bubbles and the relationship between the two follows the Richardson-Zaki prediction. For the non-Newtonian fluids the Richardson-Zaki law doesn't work. A maximum in bubble rise velocity at intermediate bubble volume fractions can be observed, while at the highest concentrations of NaSal the bubbles become trapped in the solution until coarsening sets them free.

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Wednesday 15:40 Virtual / Poster Session 2 PO34

Interfacial rheological properties of pea protein/resistant starches mixtures

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Vegetable proteins are receiving in recent years increasing attention as a functional ingredient in the food industry. They are very used to enrich of nutritional properties of soft foods, useful both for people that have feeding problems and for people interested in their own health. Pea protein, having high amino acids content, is an interesting ingredient that can impart functional properties and nutrient value to foods and for this motive is widely used in the food industry especially for gluten-free products. Pea proteins are also widely used in the production of numerous foods and the market is destined to expand rapidly in the coming years, also thanks to the increasingly massive spread of conscious food choices. The products obtained with vegetable proteins are generally enriched with starch to modulate the consistency, but one of the problems of starch addition is possible increasing of glycemia levels. So, in this work, conventional starches are substituted with resistant one due to their benefits. Resistant starches can survive to the gastrointestinal tract, then they are considered as fibres, and can favourite the well-being. On the light of the above, this work aims to obtain an optimum ratio between protein and starch and investigate the interfacial rheological properties of these mixtures to get a food structure with desired properties. Mixtures with pea protein and three different resistant starches. Interfacial measurements using the pendant drop tensiometer were performed at A/W interface. Surface tension measurements in static conditions were performed to obtain the adsorption isotherm and the CMC value both of the pea protein and the single starches; interfacial measurements in dilatational asymptotic kinematic were also performed to obtain equilibrium rheological parameters; relaxation mechanisms of analysed interfaces were also investigated in dilatational kinematic. Kinetic and rheological properties are used to get an optimum ratio between starch and pea protein concentrations.

Wednesday 15:40 Virtual / Poster Session 2 PO35

On the use of interfacial rheometers as bulk rheometers

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Interfacial shear rheometers (ISR) generally use small and light probes to shear the interface in a controlled manner. The complexity of the coupling between the interface and bulk flows has encouraged researchers to develop more refined hydrodynamical models. At the same time, the increasing computational power of regular personal computers along with autoparallelization procedures allow for the quasi-real time analysis of ISR data through the explicit calculation of the flow field at both the interface and bulk phases. Can we take advantage of these developments in interfacial rheometers to transform such devices in bulk rheometers? More explicitly, let us consider that we place our probe on a liquid/air interface, where the interface has no mechanical response and the dynamic moduli of the liquid subphase, G*, is unknown; if we acquire raw-data in such configuration, to what extent can we calculate G* from those raw-data? Our preliminary work shows that a magnetic needle ISR is capable of precisely recovering bulk viscosities as low as that of the water. The transformation of the data analysis algorithm is simple: the unknown parameter is now the bulk G*, so that the iterative procedure must be executed until the value of G* that fits the raw-data is found. Here we will report of tests of this procedure on glycerol-water mixtures, finding that the numerical scheme converges in all cases and the expected viscosity is nicely recovered. Moreover, we have extended such a procedure to similar experiments using an oscillating bicone probe attached to a rotational rheometer finding similar results. Interestingly, the same rotational rheometer can hardly measure such viscosity values using any bulk geometry and the standard analysis methods.

Wednesday 15:40 Virtual / Poster Session 2 PO36

Rheological characterization of water-based biopolymer suspensions at high temperature

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Biopolymer solutions are extensively used as rheology modifiers in environmentally friendly water-based fluids for a variety of oil field operations such as drilling, completion and enhanced oil recovery. In the most cases, these fluids are subjected to aggressive environments due to the presence of salts, high temperature and high pressure. In these conditions, rheological and physicochemical stability of the fluid is required for relatively long periods of time, in order to guaranty safe engineering operations. Cellulose nanofibers (CNF) in water suspensions show suitable properties as rheology modifiers over a wide range of temperature, since their structure and surface properties can be selected by mechanical and chemical treatments. We have characterised the rheological behaviour, as functions of pressure, temperature and concentration, of different water-based fluids, formulated with typical biopolymers (xanthan gum, CMC, etc) and CNF produced from kraft pulp paper. Oscillatory shear and viscous flow behaviour have been analysed looking for synergies between biopolymers and CNFs to formulate water-based fluids with improved rheological properties and thermal stability.

Wednesday 15:40 Virtual / Poster Session 2 PO37

Influence of thermal aging on the rheological behaviour of xanthan gum in formate brines

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Water soluble biopolymers are an interesting alternative in the oil industry to develop environmentally friendly fluids due to their biodegradability and harmlessness characteristics. Polysaccharide biopolymers have been widely used in the oilfield as viscosifiers for flooding and drilling operations due to their favorable rheology and resistance to shear degradation. Xanthan gum (XT) is preferable due to both its excellent solubility in brine solutions and its pseudoplastic behavior at low concentration and moderate temperature. These characteristics cover a wide range of engineering requirements such as high viscosity, at low shear-rate, when the flow is stopped, and low viscosity, at high shear-rate, for easy pumping circulation. Nevertheless, the structure of XT in solution degrades at high temperature, limiting the effective temperature range for engineering applications. The influence of salts on the thermo-rheological properties of XT solutions is very important to design solid-free drilling and completion fluids. Density, suitable rheological behavior and thermal resistance can be combined by controlling the type of salt and the concentration of both salt and biopolymer, where salts can act not only as weighting agent but also as thermal stabilizer. In this work, we study the influence of thermal aging on the rheological behavior of XT solutions in formate brines. We demonstrate that formate salts at high concentration protect the structure of the biopolymer against thermal degradation, retaining the rheological properties of the fluid over a wide range of temperature.

Wednesday 15:40 Virtual / Poster Session 2 PO38

Rheological, thermal and spectroscopic investigation of olive oil-based oleogels as fat phase for food emulsions

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Oleogelation is a reliable method for structuring healthy cis-unsaturated fats (which mainly composes vegetable liquid oils) to replace saturated and trans-unsaturated fats (abundant in vegetal and animal hardstocks): Their chronic consumption is believed to be dangerous for the cardiovascular apparatus of consumers. Organogelation occurs when, at a certain temperature, a relatively small amount of some specific amphiphilic compounds called oleogelators self-assembles into a 3D network via non-covalent, weak and reversible interactions such as van der Waals and H-bonding in the case of Low Molecular Weight Organogelators (LMWO). LMWOs are able to retain a large amount of oil, giving the system an overall solid-like behaviour even if they are composed of liquids for the most part and, therefore, they exhibit similar organoleptic features to widely used solid fats. Rheological (both small amplitude oscillatory and steady shear tests), thermal (Differential Scanning Calorimetry) and spectroscopic (Nuclear Magnetic Resonance, InfraRed, and Visible spectrophotometry) studies were carried out with a thermal cooling ramp on binary systems composed by olive oil and edible oleogelators (obtained from plant-based raw material processing, such as monoacylglycerols, policosanol, beeswax, Carnauba wax and Manuka wax). With the binary mixtures we were able to highlight the formation kinetics of interactions andprovide a better understanding of the link between macroscopic and microscopic variables. The overall aim was the formulation of a predictable pattern, which could be used in the fat industry to improve the technology of the process, especially in using the oleogels as the fat phase of water-in-oil emulsions: This kind of system is already being commercialised and its production technology is continuously evolving and updating.

Wednesday 15:40 Virtual / Poster Session 2 PO39

High-frequency Optimally Windowed Chirp rheometry in fast evolving systems

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Frequency-modulated excitation waveform, known as Chirp, has emerged recently as promising way to interrogate the linear viscoelastic properties of time-evolving materials. With this method the linear viscoelastic spectrum can be obtained very fast compared to classic frequency sweeps. However, the ability of the software-controlled motor of commercial rotations rheometers, to impose such a complex strain waveform has limitations. We utilize frequency- and amplitude-modulated strain waveform [1] in conjunction with a home-made sliding plate piezo-operated rheometer [2] to probe the linear viscoelasticity of time -evolving materials. The simplicity of the setup due to the absence of any kind of firmware and the microsecond actuator-sensor response prove this device an ideal case study of the advantages of this technique. The high frequency capability of this piezo-rheometer allows us to extend the accessible linear viscoelastic spectrum and most importantly, to shorten the length of the interrogating strain signal (Chirp) at a subsecond scale. Therefore the duration of the scan is short compared to the evolution of moduli (mutation time) keeping the mutation number (Nmu) [3] sufficiently low, even in fast evolving systems. To this end, we provide proof of concept, by capturing the solidification of fast evolving soft matter composites such as a vinylester resin-fumed silica nanocomposite during curing process. The sol-gel transition is captured as the LVE spectrum is accessed almost every second portraying the rapid evolution of moduli with adequate time resolution. Comparison of the Chirp utilization in commercial rotational and piezo based rheometer provides further information on the applicability of the technique. Work in collaboration with Michela Geri and Gareth H McKinley (MIT)

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Wednesday 15:40 Virtual / Poster Session 2 PO40

Jets of discontinuously shear thickening suspension

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In the present work, jets of discontinuously shear thickening (DST) suspension emerging from a vertical pipe have been experimentally studied. The suspension flows through the pipe under gravity at nearly constant flow rate and the stress field in the jet is mostly extensional with the stress levels governed by gravitational forces. The dynamics of the jet was recorded with a high-speed camera at 300 fps, then the recorded videos were discretized into pictures and carefully analyzed with an image-processing software Image J. The suspension is a concentrated mixture of calcium carbonate (CC) microparticles dispersed in water at 68% volume fraction with addition of different concentrations of polyamide (PA) microfibers of 700µm x 15 µm in size. The CC suspension solely exhibits strong DST behavior characterized by a viscosity divergence above a critical stress. At a given flow rate, depending on the jet length (distance between the pipe outlet and a point where the jet hits the experimental table), different behaviors are observed varying between stable viscous thread to coiling instability and elastic instabilities with periodic rupturing of the jet ascribed to achievement of the critical stress of the DST onset under extensional deformations. Addition of fibers mainly stabilizes the jets and this effect is still not fully understood and perhaps depends on the flow-induced orientation of fibers under extensional flow, increasing extensional viscosity. In this communication we will discuss in detail different regimes and present experimental correlations between the fiber concentration and dynamic parameters of the jet instability (wavelengths, lateral oscillation amplitudes, etc.) The results of this work are believed to be helpful in the field of fiber-reinforced cementitious materials.

Wednesday 15:40 Virtual / Poster Session 2 PO41

Neural networks for modelling creep stress-strain relation at different temperatures

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Our previous research showed that neural networks (NN) are useful for solving inverse problems for obtaining material function from non-standard excitation in the presence of noise. Therefore, we further investigate their applicability for real-time structural health monitoring of polymer-based structures. NN's main advantage is that they can be trained to detect changes in structural response related to material property change due to environmental conditions (temperature, humidity) and time. Unfortunately, currently used structural health monitoring systems deal mostly with geometrical changes (cracks, delamination) and do not consider temperature-, humidity- or the matrix material's time-dependency. In our past work, we have shown the Multilayer Perceptron (MLP) neural network capabilities to solve an ill-posed inverse problem to determine creep compliance. This paper represents the next step of the research and focuses on the application of MLP for modelling the material behavior on real experimental data. Polyether ether ketone (PEEK) was selected as high-performance material utilized in the aerospace industry due to its superior mechanical and thermal properties. Constant shear stress rate tests were performed at different temperatures using a rotational rheometer. Obtained stress-strain data was utilized for training MLP. The experimental procedure for training data generation and neural network design steps, including training procedure, choice of data for better generalization and topology optimization, is presented within the paper. We have shown that proper choice of temperatures corresponding to training data is of crucial importance and demonstrated that one layer MLP trained with Bayesian generalization algorithm can provide satisfactory prediction and generalization results.

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Wednesday 15:40 Virtual / Poster Session 2 PO42

Effect of ethylene-bis-stearamide wax on the rheological properties of SAN and ABS copolymers

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Ethylene-Bis-Stearamide (EBS) is a synthetic wax used as lubricant for thermoplastic polymers. In this study the solubility and plasticization of this additive in SAN and ABS copolymers was investigated by means of rheological measurements performed with a capillary rheometer in a wide concentration and temperature range. Rheology proves to be not only a powerful but also an essential tool in this specific case because this wax melts above the glass transition temperature of the thermoplastc matrix and crystallization on cooling clearly results in phase separation of the additive. Solubility limits and a temperature dependent phase diagram were obtained. Exploiting a temperature-concentration superposition effect the preferential distribution of the additive in the rubbery phase of ABS copolymers could be demonstrated and quantified. The phase diagram obtained shows a linear dependent temperature of solubility with increasing amount of EBS wax disperded. Flow curves of highly concentrated blends also reveal the existence of stress induced mixing/demixing phenomena.

Wednesday 15:40 Virtual / Poster Session 2 PO43

Capillary pressure dynamometry for the characterization of polymeric membranes at liquid interfaces

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The characterisation of the visco-elastic properties of interfaces arising in foams and emulsions is of primordial importance to understand and optimise their overall properties. A wide range of techniques exist to characterise reliably the dilational or shear properties of fluid-like interfaces. However, with the increasingly popular use of foams and emulsions with solid-like, visco-elastic interfaces, new approaches are required and under the development. Here we use pressure measurements (capillary pressure dynamometry) of nearly spherical, oscillating bubbles and drops held by a needle to determine the visco-elastic properties of solid-like, visco-elastic interfaces composed of different types of polymers. Examples include interfaces composed of polyelectrolyte multi-layers (NaPSS/PAH), gels of alginates or silicones. In the case of a bubble whose surface area A is varied sinusoidally around a reference value A0 while a polymeric layer is grown on its surface it is possible to observe that surface tention decrises. We combine a classic shape tensiometry with pressure dynamometry to acces the mechanical behaviour of the interface. In the latter one notices the evolution from the interface being a "visco-elastic fluid" (presure decreases when the deformation increases) to one where the interface is a "visco-elastic solid" (presure increases with deformation; and where the tensiometry become erroneous) via a change of slope of the pressure variation with A/A0. Using different types of classic polymer models (Neo-Hooke, Hooke, etc.), we analyse the error induced by the presence of the needle and we deduce the visco-elastic moduli of the polymeric layer in comparison to the bulk properties of these polymers.

Wednesday 15:40 Virtual / Poster Session 2 PO44

Tweezing self-assembled objects: from colloidal membranes to twisted ribbons

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Viruses as model colloids, tweezing self-assembled objects Filamentous bacteriophages such as fd-like viruses are monodisperse rod-like colloids that have well defined properties of diameter, length, rigidity, charge and chirality. Such viruses, and the mutant fd-y21m in particular, can be considered as model rigid rods in the framework defined by Onsager to capture the isotropic nematic transition. Their condensation in an aqueous solution with additive polymers, which act as depletants to induce attraction between the rods, leads to a myriad of fluid-like micronic structures. I will focus on the transition between two such structures, colloidal membranes and twisted ribbons, using laser tweezers.

Wednesday 15:40 Virtual / Poster Session 2 PO45

k-carrageenan/PVA hydrogels as a bio-ink for cartilage reconstruction

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The design of biologically active scaffolds with suitable characteristics is one of the key factors for the success of tissue engineering. Many researches have shown that cells cultured in vitro in 3D resemble the physiology of their counterparts in vivo much better than cells cultured conventionally on flat surfaces of tissue culture plates. Hydrogels have received a considerable interest as leading candidates for engineered tissue scaffolds due to their unique compositional and similarities to the natural extracellular matrix. In addition to their porous structure allows the incorporation of growth factors, glycans, bioactive peptides and natural proteins necessary for cell proliferation and survival. Most recently, 3D bio-printing, using a mixture of cells, biopolymers and bioactive molecules, has received particular attention due to the possibility of placing the cells in the right positions inside the matrix structure to create complex biohybrid structures. Human adipose-derived stem cells (hADSCs) spheroids are relatively accessible and attractive as a cell source for cartilage regeneration, due to the simple surgical procedures required to harvest the cells, the repeatable access to the subcutaneous adipose tissue and relatively easy enzyme-based isolation procedures. In the present work we have prepared and characterized different hydrogel blends composed by k-carrageenan (k-C) and PVA. Their mechanical and morphological properties, as well as their degradation behavior have been characterized, in the prospect of using them as a 3D bio-matrix in which hADSCs can be seeded for cartilage reconstruction.

Wednesday 15:40 Virtual / Poster Session 2 PO46

The effect of drugs rheological properties in the flow accuracy and uncertainty of infusion systems within the microflow range

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In clinical treatments most of the drug solutions used in multi-infusion systems are water-based solutions behaving like ideal viscous liquids and therefore behaving as Newtonian liquids when under flow. However, when the perfusion occurs within the µL/min range, some of the drugs with more complex composition, such as protein or particle-based, shown viscoelastic flow behaviour, meaning that their viscosity depends on the flow rate imposed. This is the case of propofol, the drug used almost always to induce general anesthesia by using manually programmed infusion pumps or computer-controlled infusion pumps in a process called target controlled infusion (TCI). However, even though perfusion systems are widely used in therapeutics to infuse a multitude of drugs, few are the published studies about the influence of drugs physical properties, namely rheological, on the accuracy and uncertainty of the flow rate of these instruments. So, the European joint research project EMPIR Metrology for Drug Delivery (MeDD II) is now focused on providing traceable measurements of volume, flow and pressure of existing drug delivery devices and mixing behavior and occlusion phenomena in multi-infusion systems. In addition to propofol, also Gelaspan®, a colloidal plasma volume substitute was also tested, at very low flow rates. So, the purpose of this communication is to give more insight regarding the effect of drugs rheological properties in the flow accuracy and uncertainty of infusion systems within the flow rate range from 1 to 1000 µL/min.

Wednesday 15:40 Virtual / Poster Session 2 PO47

Dynamic shear rheological properties of highly filled composites for additive manufacturing

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One of the major applications of highly filled polymers with more than 40 vol.% of fillers is the indirect fabrication of metal, ceramic, or cermet parts with complex geometry in powder injection moulding, powder extrusion moulding, and more recently, powder fused filament fabrication (PFFF). The rheological behaviour of highly filled materials is complex and influenced by many interrelated factors. In the present study, we considered four different spherical filler materials: steel, aluminium alloy, titanium alloy and glass beads. To obtain highly filled composites, the particles with similar particle size distribution were mixed with a polypropylene-based binder system at different filling grades (30-60 vol.%). The presented research results proved that the rheological behaviour of highly filled composites strongly depends on the interactions between the filler and matrix material, assuming that the same matrix material is used and that the filler material size and shape remain the same. In this particular case, the steel and aluminium particles formed chemical bonds between the particles and the matrix, and as such the rheological values were higher than the fillers forming physical interactions only (i.e., titanium alloy and glass beads). Moreover, it was shown that processing conditions could change the particle shape and size resulting in unexpected rheological behaviour of composite materials. Such effect was observed in the composites filled with high concentrations of glass beads that broke during processing which significantly altered the rheological behaviour.

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Wednesday 15:40 Virtual / Poster Session 2 PO48

Rheometry of complex liquid/liquid interfaces using millifluidic extensional flow

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Multiphasic fluids are ubiquitous in daily life and industrial processes. Among them, emulsions, foams, droplets or bubbles have mechanical, isolation and exchange properties, which can be useful to design final products. However, multiphase fluid stability is an issue since coarsening and/or coalescence lead to the ageing of the product and significantly modify its initial properties. Using surface-active materials which adsorb onto interfaces such as surfactants, polymers, proteins or particles, is a way to hinder such unwanted ageing effects. Unfortunately, selecting efficient surface agents to stabilize droplets and bubbles is still based on an experimental know-how rather than on a global understanding. The goal of our project is to quantify the mechanical properties of the interfaces to provide a clearer frame to this problem.

Using millifluidic extensional flow, we measure the maximum deformation of a water in oil droplet under different flow conditions and we extract the effective interfacial tension. We observe that this surface tension strongly depends on the surfactant concentration and is different from the surface tension at rest, especially around the CMC.

Hereby, we propose a non intrusive way to characterize indirectly the mechanical properties of the interfaces of complex multiphasic fluids. Through varying surfactant concentration, we can bring to light the influence of surfactant dynamics on the liquid/liquid interface stability. This should help in choosing, in an effective way, the amount and the nature of a surfactant depending on the constraints of an application.

Wednesday 15:40 Virtual / Poster Session 2 PO49

Wetting of yield stress fluids

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When a liquid drop is gently deposited on a wetting solid surface, it spreads due to capillary forces until it reaches a thermodynamical equilibrium set by the relative surface energies of the system. We investigate here experimentally the spreading ability of drops made of yield stress fluids, which flow only if the applied stress is above a finite value. We observe that in this case, after a spreading phase, the motion stops and a well-defined contact angle can be measured. This contact angle depends on the rheological properties of the fluid and in particular on its yield stress, on the drop radius and on the hydrodynamic boundary condition at the surface. These results are quantitatively compared to an analysis showing that, due to the yield stress of the fluid, a mechanical equilibrium is indeed reached which does not correspond to the thermodynamical equilibrium.

Wednesday 15:40 Virtual / Poster Session 2 PO50

Swimming bacterial in biofilms under shear flow

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Biofilms are surface-attached microbial systems, whose formation is strongly affected by environmental conditions such as chemical and mechanical stimuli such as shear stress (Lecuyer, New. J. Phys. 2015, Rusconi, Ann. Rev. Biophys. 2014, Persant, Cells 2015), by inducing bacterial attachment on solid surfaces and the subsequent biofilm development. A full comprehension of the complexity of cells behaviour towards mechanical cues is not yet understood. The role of the shear stress on bacterial cells motility in biofilm is here investigated. Pseudomonas fluorescens biofilms are cultivated under laminar flow conditions using a commercial microfluidic device integrated in a custom-made Time Lapse microscopy workstation equipped with a fast camera. The experimental apparatus is capable to operate with limited operative volumes with a large surface/volume ratio, which enhances mass transport within biological systems, and achieves stable shear flow conditions by simply tailoring the hydrodynamic conditions (Di Somma, J Mol Sci 2020, Recupido, Coll. Surf. B 2020). Trajectories described by cells under flow are reconstructed by Image Analysis and analysed according to motility models available in the literature. Isotropic (Dickinson & Tranquillo, 1995, Bioengineering, Food and Natural Products) and anisotropic (Wirz et al., 2011, Nat Rev Cancer.) persistent random walk models have been considered, calculating motility parameters from cell mean square displacement measurements as function of time. Cell speed, persistence time, and random motility coefficient have been obtained as function of the flow intensity. Bacteria swim in the biofilm, moving with different velocity respect to the imposed flow profile. The degree of development of biofilm influences the motility of bacteria.

Wednesday 15:40 Virtual / Poster Session 2 PO51

Role of flow-induced stress in cancer growth and invasion

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Cancer is a complex, heterogeneous, multifactorial, and multistage disease, that is a leading healthcare problem worldwide, and is currently the second cause of death, following cardiovascular diseases, in advanced countries. Several experimental and clinical studies of malignant neoplasms indicate that invasive growth and metastasis are the main manifestations of tumour progression. Tumours invasion is strongly influenced by the microenvironment and, among other parameters, mechanical stresses play an important role. This work is focused on the development and validation of innovative methodologies to measure the role of external (bio-)mechanical stimuli on the capacity of tumours to invade the surrounding healthy tissue, using a 3D model of not-vascularised tumour: the spheroid. Tumoral spheroids are tightly bound cellular aggregates that tend to form when transformed cells are maintained under nonadherent conditions. To quantify the influence of external stimuli on tumour, we apply a shear flow to the spheroids, using a microfluidic device. Spheroids are suspended in a modified medium, formulated by adding polyvinylpyrrolidone (PVP) to standard culture medium, to increase the viscosity, minimize spheroids sedimentation, and increase shear stress. The morphology response (i.e. deformation) of tumour spheroids in flow can be analysed in analogy with a multiphase fluid following the classical approach proposed by Taylor. The analysis allows to estimate cell-cell attractive forces within the spheroid, that are related to tumour invasiveness toward the surrounding tissue. The experimental results obtained by the study of in-vitro models (spheroids), are here also compared to predictions obtained from in-silico models, based on a chemical engineering approach, focusing on the role of transport phenomena. The numerical model was developed using a hybrid approach that couples continuous analysis with finite elements codes.

Wednesday 15:40 Virtual / Poster Session 2 PO52

Gaining insight on the rheological percolation concept of polymer based nanocomposites

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The following equation, derived from the statistical percolation theory, $X=X_0\ (\Phi-\Phi_c)$^t (Eq 1) where X is the physical property under evaluation, φ the nanoparticles concentration, Φ_c the percolation threshold and t an adjustable parameter, has been profusely used to evaluate the percolation threshold in polymer nanocomposites. In the majority of the cases the contemplated X property is the electrical conductivity, s, which allows calculating the electrical percolation threshold in polymer composites that contain electrical conductive particles, such as carbon black, or conductive nanoparticles like carbon nanotubes, CNT, or graphene. Eq 1 has also been employed to determine a rheological percolation threshold using data obtained in the linear viscoelastic regime by SAOS measurements. For instance, the elastic modulus, G', measured at low frequencies has been considered [1] taking X=G' in Eq 1, but the physical interpretation of the obtained Φ_c remains rather imprecise. In this work we propose a new method to obtain the rheological percolation threshold and define its physical meaning more precisely. The experimentally contemplated systems are nanocomposites based on polymer matrices, such as polypropylene, PP, and polyurethanes, PU, filled by CNT particles. The proposed rheological tool is deduced from SAOS results, considering phase angle as a function of complex modulus G* [2,3]. The analysis of a phase angle maximum observed in nanocomposites (but not in pure polymers) as frequency is decreased, allows defining a transition from the restriction imposed by entanglements to the restriction imparted by the polymer/nanoparticles network. Deepening in this concept we deduce that Φ_c would correspond to the concentration value for the minimum distance between polymer/CNT interactions to create a rheologicaly effective network.

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Wednesday 15:40 Virtual / Poster Session 2 PO53

Effects of NaCl and alginate concentrations on the rheological properties of aqueous solutions and hydrogels

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Sodium alginate based hydrogels are an appealing candidate for in vitro models of mucus. They proved effective in reproducing the mechanical properties and diffusivity of both physiological and pathological pulmonary mucus [1]. However, extension of its use in other body districts with different physiological salt concentration, or its use in presence of culture mediums for bacteria/cells growth requires a redesign of the hydrogel. This involves the identification of the appropriate concentration of the precursor alginate solution along with the definition of the proper crosslinking conditions. At present, this process requires a time-consuming trial and error approach. However, some evidence suggest that a correlation exists between the rheological behaviors of the precursor solution and hydrogel: this would allow the tuning of the mucus model by formulating the precursor solution before the gel production. As a preliminary step to the definition of these correlation, we present a systematic investigation of the effect of NaCl content and alginate concentration on the rheological behavior of relevant solutions. The alginate concentration increases the solution viscosity at constant salt content, and the effect can be interpreted based on the scaling theory for polyelectrolytes [2]. In its turn, NaCl content has a strong effect on solution viscosity, reducing it below 2% w/v concentration and increasing it above this value. In agreement with theoretical predictions, scaling laws in this case get closer to those of a neutral polymer [3]. Finally, a significant effect of the solution preparation procedure was observed, indicating that the conformations of the chains of sodium alginate are strongly affected by the ionic strength of the solvent, and not only by that of the final solution. This aspect is currently under investigation.

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Wednesday 15:40 Virtual / Poster Session 2 PO54

Tribology as a tool to evaluate the lubricant performance of dressings used by healthcare professionals during the COVID-19 pandemic

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The COVID-19 pandemic enforced the use of personal protective equipment (PPE), especially by healthcare professionals (HCPs). The prolonged use of PPEs causes constant frictional and pressure forces on skin tissues, causing lesions. Semipermeable, padded and hydrocolloid dressings, placed between the skin and the PPE, are being widely used as a protective barrier. The aim of this study was to evaluate the lubricant properties of different dressings in different conditions, using tribology, to assess if such dressings provide an efficient protective barrier to prevent skin lesions in HCPs. In this study three of the most widely used types of dressings which HCPs use underneath the PPE, namely a hydrofiber (Fibrosol®, Pharmaplast), a silicon (Silicone Net, Innomed) and a developed gelatine-based hydrogel dressing, were evaluated using tribology. To assess the lubrication process, a constant force was applied at different velocities using a controlled stress Malvern Kinexus Lab+ Rheometer equipment (Malvern, UK) with a three-ball-on-plate tribometer geometry in rotational mode. Two forces were tested, 0.5N (surgical masks use simulation) and 1.5N (FFP2 use simulation), in the presence or absence of sweat. The results obtained revealed that both commercial dressings presented low friction values in both with and without sweat conditions tested, meaning their properties are preserved even in the presence of sweat. The gelatin-based hydrogel presented lower friction values in the presence of sweat in comparison with non-sweat conditions, showing a similar behaviour to the commercially available dressings.This result suggests that the hydrogel dressing has good lubricant properties. In conclusion, tribology revealed to be a useful tool to evaluate the lubricant capacity of dressings to prevent skin lesions in HCPs. Ongoing studies with other excipients and conditions, such as body temperature simulation, are being tested to achieve an improved hydrogel dressing with lubricant properties.

Wednesday 15:40 Virtual / Poster Session 2 PO55

The effect of blood and red blood cells viscoelasticity on microcirculation

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Blood is a complex fluid that is primarily composed of red blood cells (RBCs), which occupy about 45% (hematocrit, Hct) of human blood volume, suspended in plasma, a liquid rich of low and highmolecular weight species, such as electrolytes, hormones, clotting factors and proteins. In turn, RBCs have a complex mechanical behavior, which can be described in terms of their deformability and aggregation, promoted by the presence of plasma proteins, primarily fibrinogen, as well as by the addition of macromolecules as dextran. Indeed, the tendency of RBCs to form packed structures plays an important role in blood flow behavior, causing the increase of blood viscosity, especially at low shear rates. Two main models have been proposed so far to describe RBC aggregation: the bridging model, based on the assumption that macromolecules as fibrinogen or dextran act as a bridge between two adjacent RBCs, and the depletion model, based on the osmotic pressure due to the presence of macromolecules in the suspending medium, leading to depletion interaction. Nevertheless, the mechanism at the base of RBC aggregation is controversial and not yet fully elucidated. Here, we present an overview of blood and RBCs viscoelastic properties and their effect on blood microcirculation. Blood viscoelasticity has been investigated by by conventional bulk rheology in the linear viscoelastic regime, finding that G" predominates over G' across the entire tested range of frequency. The effects of RBC volume fraction and of aggregating media (i.e., dextran solution at two different concentrations) have been also investigated. RBC membrane rheological behavior has been investigated by analyzing the transient behavior of RBC shape in confined flow and by measuring the membrane viscoelastic properties in converging/diverging microchannels. Possible applications include the analysis of RBC deformability and aggregation in pathological situations, for which reliable quantitative methods are still lacking.

Wednesday 15:40 Virtual / Poster Session 2 PO56

Investigation of the yielding transition in concentrated colloidal systems via rheo-XPCS

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We probe the microstructural yielding dynamics of a concentrated colloidal system by performing creep/recovery tests with simultaneous collection of scattering data via X-ray Photon Correlation Spectroscopy (XPCS). This combination of rheology and scattering allows for time-resolved observations of the microstructural dynamics as yielding occurs, which can be linked back to the applied rheological deformation to form structure-property relations. To more accurately track the non-equilibrium processes which occur under yielding, we utilize two-time correlation functions, which provide additional time-resolved information that is inaccessible via more typical one-time correlations. Under sufficiently small

applied creep stresses, examination of the correlation in the flow direction reveals that the scattering response recorrelates with its pre-deformed state, indicating nearly-complete microstructural recovery. Conversely, larger creep stresses increase the speed of the dynamics under both applied creep and recovery. The data show a strong connection between the microstructural dynamics and the acquisition of unrecoverable strain. By comparing this relationship to that predicted from homogeneous, affine shearing, we find that the yielding transition of concentrated colloidal systems is highly heterogenous on the microstructural level.

Wednesday 15:40 Virtual / Poster Session 2 PO57

Doppler methods as useful tool for non-newtonian fluids rheological properties detecting during flow

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The aim of the research was to develop the ultrasonic measuring method dedicated to fluids under real flow through the pipeline. The measurement system is a set of appropriately configured ultrasonic heads and pressure sensors installed on the pipeline. Based on the attitude of sound propagation measurements inside fluid, it is possible to obtain information on the velocity profile in the pipeline cross-section. These data in combination with the pressure drop values detected on the measuring section are sufficient to clearly determine the rheological properties of the fluid. The measuring system used for the tests consisted of a screw pump, two pressure sensors, an electromagnetic flow meter and four ultrasonic heads. The length of the measuring section was 4 m, and the internal diameter of the pipeline was 0.025 m. To calibrate of measurement system glycerol was used. As a model fluid, a 1% water solution of xanthan gum was used and was subjected to the flow at following shear rate conditions: 5, 11, 17, 23, 29, 35, 41, 47 s^{-1}. The raw experimental data obtained were the Doppler frequences. They were recalculated to velocity profiles and with pressure drop values created a full information about fluid behavior during flow. According to momentum balance equation and thixotropic pseud-mass balance (Kemblowski-Petera theory) the rheological parameters of Ostwald de Waele model were estimated. The estimation procedure was carried out with the help of Marquardt-Levenberg minimisation method. The same solutions were tested with the help of rotational rheometer. The data obtained form Doppler and pressure drop methods were consistent with the results obtained from the rotational rheometer. The use of Doppler methods and measurement of pressure drop allows to determine the rheological properties of the non-newtonian fluids under the process conditions directly in the pipeline. In addition, it is possible to perform full rheological characteristics based on one flow rate under laminar conditions.

Wednesday 15:40 Virtual / Poster Session 2 PO58

Evolution of the appearance of liquid-crystalline textures of calf-thymus DNA under flow in the entanglement regime

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DNA's ability to form liquid crystal phases has been known for many years. Liquid crystal ordering appears as a general form of natural ordering in DNA solutions at specific conditions, i.e. DNA molecular weight, DNA concentration and external salt concentration. DNA solutions can form liquid crystalline phases over a critical concentration of polymer. Moreover, shear-induced crystalline textures induced by flow in calf-thymus DNA (for 7 and 10 mg/mL), were recently revealed through local birefringence measurements and visualizations, coupled with rheological measurements. In this work, we studied calf thymus DNA molecules organization under flow in the entanglement regime, using rheological measurements. Dynamic and flow measurements were carried on for DNA solutions having concentrations between 4 to 15 mg/mL at a pH of 7.4 and at a temperature of 20 °C. Visual observations between crossed polarizers allowed detecting the appearance of shear-induced birefringence for all DNA solutions. Then, the appearance of a shear stress plateau, from a DNA concentration of 7 mg/mL was observed in the shear stress curves. The critical shear rate at which the plateau appears decreases with the increase in DNA concentration. The origin of this plateau was related to the presence of crystalline textured DNA clusters that get oriented in the flow. The critical shear rates, corresponding to different transitions observed in the flow curve for each DNA concentration, from 7 to 15 mg/mL, allowed proposing a phase diagram in terms of shear stress as a function of DNA concentration. In this phase diagram it is possible to identify a zone of DNA chains reorganization, followed by the entrance to the crystalline texture formation zone, in which the amorphous parts of DNA chains are progressively stretched and orientated in the flow, and the zone of complete orientation of the DNA chains forming a uniform anisotropic monodomain, related to a pseudo-nematic phase, which appears at higher shear rates as DNA concentration increases.

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