

Book of Abstracts



10th International Conference of the *Hellenic Society of Rheology*

*Honoring Professor Pino Marrucci and Professor Evan Mitsoulis
for their contributions to Rheology*

29 June – 2 July, 2022

Skiathos, Greece

Sponsor



Message from the organizers

It is with great pleasure that we welcome all the delegates and accompanying persons to the 10th International Meeting of the Hellenic Society of Rheology (*HSR2022*), Skiathos, June 29 - July 2, 2022.

The 1st meeting of the HSR took place in Nicosia, Cyprus, in 1996. Since then, the HSR meetings took place in Heraklion (1998 and 2014), Patras (2001), Athens (2004 and 2011), Rhodes (2007), in Limassol (2017), and in Samos (2019). The main goal of these meetings is to promote scientific interactions at the highest level not only among the members of the Greek Chapter of the Society of Rheology but also among scientists from all over the World. Another objective of the meetings is to provide the forum where students could interact and share their work with the established members of the community.

HSR2022 is devoted to Professor Pino Marrucci and Professor Evan Mitsoulis for their contributions to rheology. Professor Evan Mitsoulis was a founding member and served as the first President of HSR (1996-1998).

The program includes three invited keynote talks by Professors Pino Marrucci (University of Naples, Italy), Evan Mitsoulis (National Technical University of Athens, Greece), and Paula Moldenaers (Katholieke Universiteit Leuven, Belgium), 34 regular talks, and 11 poster presentations. A short course on ***Non-Equilibrium Thermodynamics Modeling of the Rheology and Transport Phenomena***, offered by Professor Antony N. Beris (University of Delaware), preceded the conference on June 29, 2022.

With approximately 50 registered participants from 13 countries (Austria, Belgium, Canada, Cyprus, Germany, Greece, Italy, Israel, Slovenia, Sweden, Switzerland, UK, and USA) the conference is truly an international event.

We hope that *HSR2022* will promote scientific exchange, collaboration and interactions between participants.

Nikos Pelekasis
University of Thessaly

Georgios Georgiou
University of Cyprus

HSR2022 PROGRAM

Conference Venue: Skiathos Palace Hotel, Koukounaries, Skiathos

Wednesday, June 29, 2022

Short course

Non-Equilibrium Thermodynamics Modeling of the Rheology and Transport Phenomena

Instructor: Professor Antony N. Beris (University of Delaware)

08:00-08:30	Reception & Registration
08:30-12:20	4 x 50' lectures followed by 10' breaks
12:20-14:10	Lunch Break
14:10-16:00	2 x 50' lectures with a 10' break
16:00	End of short course

HSR2022 Conference

16:00-19:00	Registration
18:00-19:00	Poster Session - Committee: Stavroula Balabani, Savvas G. Hatzikiriakos
18:00-19:00	<p>Th. Athanasiou, M. Geri, G. McKinley, G. Petekidis, <i>High-frequency Optimally Windowed Chirp rheometry in fast evolving thermosets</i></p> <p>N.A. Burger, G. Meier, L. Bouteiller, B. Loppinet, D. Vlassopoulos, <i>High-pressure microrheology of supramolecular assemblies</i></p> <p>A. Diligenza, G. Esposito, K. Giannokostas, Y. Dimakopoulos, J. Tsamopoulos, <i>Hematocrit level-based assessment of turbulent-related wall shear stress of pulsatile blood flow in a pathological coarctation of the human aorta</i></p> <p>G.C. Florides, M. Modigell, G.C. Georgiou, E.J. Zoqui, <i>Squeeze flow of thixotropic semisolid slurries</i></p> <p>S.D. Gkormpatsis, K.D. Housiadas, G.C. Georgiou, <i>Steady sphere translation in an Oldroyd-B fluid with non-linear slip on the surface of the sphere</i></p> <p>E. Gryparis, C. Xenophontos, G.C. Georgiou, <i>Torsional parallel plate flow of Herschel-Bulkley fluids with wall slip</i></p> <p>N. Pelekasis, M. Vlachomitrou, A. Lytra, D. Dimopoulos, <i>Numerical study of the dynamic response of a liquid metal in a pore in the presence of a magnetic field and a heat load</i></p> <p>E. Moghimi, D. Vlassopoulos, <i>Rheology of reversible networks from star block copolymers</i></p> <p>A. Oikonomou, V. Vaitsis, M. Vlachomitrou, N. Pelekasis, <i>Trapped pulsations of microbubbles near a wall: Effect of sound amplitude and liquid viscosity on the microstreaming pattern</i></p> <p>S. Rosios, N. Pelekasis, <i>Weakly nonlinear analysis of the effect of shell stiffness on the fundamental resonance of coated microbubbles</i></p> <p>E. Vereroudakis, V. Chrisoulaki, E. Moghimi, G. Petekidis, <i>Crystallizing depletion colloidal gels by shear</i></p>
19:00-21:30	Transport and Welcome Reception at Agia Eleni Beach

Thursday, June 30, 2022

08:00-08:30	Registration
	Chair: Giovanni Ianniruberto
08:30-08:40	Opening, Introduction of Honoree Giuseppe Marrucci by Antony Beris
08:40-09:20	G. Marrucci , G. Ianniruberto, <i>Fast flows of unentangled polymers</i>
09:20-10:00	C. Schaefer, T.C.B. McLeish , <i>Spinning a yarn of the molecular rheology of natural silk spinning: sticky reptation in extensional flow</i>
10:00-10:20	C. Carotenuto, M. Minale , <i>Microstructural changes of concentrated Newtonian non-Brownian suspensions under oscillatory shear originating the failure of Cox-Merz rule</i>
10:20-10:40	T. Athanasiou, S. Kamble, D. Parisi, T. Chang, J. Allgaier, D. Richter, D. Vlassopoulos , <i>Ring polymer rheology and the limits of experimentation</i>
10:40-11:00	Coffee break
	Chair: Stavroula Balabani
11:00-11:20	D. Kogan, M. Gottlieb , <i>Non-linear-viscoelasticity characteristics of the gelation process</i>
11:20-11:40	S. Costanzo , V. Ianniello, <i>Nonlinear shear rheology of nearly unentangled H-polymer melts and solutions</i>
11:40-12:00	J. Piette, A.A. Moud, S.G. Hatzikiriakos , <i>Rheology of mature fine tailings</i>
12:00-12:20	S. Mitrou , S. Migliozzi, P. Angeli, L. Mazzei, <i>Rheology of dilute polydisperse bubble suspensions</i>
12:20-12:40	T. Athanasiou , N. Kalafatakis, D. Vlassopoulos, <i>Measurement of both normal stress differences using two partitions and piezoelectric sensor</i>
12:40-14:00	Lunch break
	Chair: Pavlos S. Stephanou
14:00-14:20	P. Moschopoulos , S. Varchanis, A. Syrakos, Y. Dimakopoulos, J. Tsamopoulos, <i>S-PAL: A stabilized finite element formulation for computing viscoplastic flows</i>
14:20-14:40	C. Pseudos, K. Giannokostas, Y. Dimakopoulos , J. Tsamopoulos, <i>A monophasic blood flow model for accurate prediction of wall shear stresses in the microcirculation</i>
14:40-15:00	D. Pasias, E. Kaliviotis , <i>Blood viscosity in passive microchannel flows: effects of erythrocyte deformability, aggregation and haematocrit</i>
15:00-15:20	M. Vlachomitrou , N. Pelekasis, <i>Acoustic interrogation of coated microbubbles in a wall restricted flow: the compression only and microstreaming effects</i>
15:20-15:40	A. Marousis, K. Psaraki, Y. Dimakopoulos , J. Tsamopoulos, <i>A multiphase model of vascular smooth muscle cell</i>
15:40-16:00	Coffee break
	Chair: Yannis Dimakopoulos
16:00-16:20	J. Bergfreund, P. Bertsch, P. Fischer , <i>Role of the hydrophobic phase on interfacial phenomena of surfactants, proteins, and particles at fluid interfaces</i>
16:20-16:40	T.X.D. Nguyen, S. Razavi, D.V. Papavassiliou , <i>Effects of surface-active nanoparticles and surfactants on the migration of drops in nanochannels</i>
16:40-17:00	A. Katsiavria , D.T. Papageorgiou, <i>Novel instabilities in immiscible multilayer viscous shear flows in the presence of interfacial slip</i>
17:00-17:20	A. Lytra , M. Vlachomitrou, N. Pelekasis, <i>Steady state and dynamic simulations of axisymmetric gas-liquid flow focusing arrangement in the presence of surfactants</i>
17:20	End of session - Free afternoon
21:00-24:00	HSR2022 Banquet at the Skiathos Palace Roof Garden

Friday, July 1, 2022	
	Chair: Kostas D. Housiadas
08:30-09:10	E. Mitsoulis , <i>Advances in rheology and polymer processing: A modeling and simulation point of view</i>
09:10-09:30	C. Dritselis, G. Karapetsas , <i>A parametric study of dynamics of liquid lens spreading over a viscoplastic liquid substrate</i>
09:30-09:50	A. Spyridakis , P. Moschopoulos, S. Varchanis, Y. Dimakopoulos, J. Tsamopoulos, <i>Bubble rise in elastoviscoplastic materials</i>
09:50-10:10	C. Lambride, A. Syrakos, G.C. Georgiou , <i>Flow development of power-law fluids in tubes and channels</i>
10:10-10:30	E. Vereroudakis , E. Locatelli, B. Loppinet, C. Likos, D. Vlassopoulos, <i>Study of dendronized polymers across different length scales and concentration regimes: State of the art and future perspectives</i>
10:30-10:50	Coffee break
	Chair: Efstathios Kaliviotis
10:50-11:10	N.D. Polychronopoulos , J. Vlachopoulos, <i>Extensions of Frenkel's model of viscous sintering</i>
11:10-11:30	I.N. Besiri , T.B. Goudoulas, E. Fattahi, T. Becker, <i>In situ custom-made rheological setup for real-time mechanical characterization of crosslinking reactions</i>
11:30-11:50	T. Boulafentis , T. Lacassagne, N. Cagney, S. Balabani, <i>Flame-patterns and diwhirls in elasto-inertial Taylor Couette flows</i>
11:50-12:10	A. Oseli, T. Tomković, M. Mihelčič, S.G. Hatzikiriakos, A. Vesel, L. Slemenik Perše , <i>Network formation in carbon nanotube polymer-based nanocomposites during injection and compression molding</i>
12:10-12:30	A.A. Mishra , D. Arlov, F. Innings, R. Kadar, <i>Thixotropic modelling of yield stress fluids</i>
12:30	End of morning sessions
12:30-13:30	HSR elections
13:30-15:30	Lunch break
15:30-21:30	Boat trip between Skiathos and South-East Pelion with a stop at Katigiorgi

Saturday, July 2, 2022

	Chair: Panagiota Angeli
08:30-09:10	P. Moldenaers , <i>Towards miniaturization: how does confinement affect the break-up and coalescence of droplets in shear flow?</i>
09:10-09:30	S. Jariwala, N.J. Wagner, A.N. Beris , <i>A thermodynamically consistent, microscopically-based, model of the rheology of aggregating particles suspensions</i>
09:30-09:50	D.G. Tsalikis , C. Christopoulou, K.S. Karadima, I.P. Stott, V.G. Mavrantzas, <i>Multi-scale simulation approach to morphology and microrheology of mixed surfactant-cosurfactant micellar solutions</i>
09:50-10:10	T. Athanasiou, B. Mei, K.S. Schweizer, G. Petekidis , <i>Cage formation and dynamics in repulsive and attractive glasses probed by high frequency rheology</i>
10:10-10:30	N. Antonova , <i>Evaluation of the microrheological properties of blood cells using microfluidic methods</i>
10:30-10:50	Coffee break
	Chair: Athanasios Papathanasiou
10:50-11:10	N. Patsalidis , G. Papamokos, G. Floudas, V. Harmandaris, <i>Modelling of Polymer/Alumina Interfaces via Ab-initio Calculations and Machine-learned Molecular Dynamics Simulations</i>
11:10-11:30	K. Ritos , <i>Exploring quenchant properties at the nanoscale – A molecular dynamics study</i>
11:30-11:50	E. Gkolfi , P. Bacova, V. Harmandaris, <i>Investigation of the tunable character of the star-shaped polymer melts through chemistry-specific model</i>
11:50-12:10	P.S. Stephanou , I.Ch. Tsimouri, V.G. Mavrantzas, <i>A two-species model for the rheology of associative polymer networks from nonequilibrium thermodynamics</i>
12:10	Closing Remarks: Nikos Pelekasis and Kostas Housiadas

INVITED TALKS

Fast flows of unentangled polymers

Giuseppe Marrucci and Giovanni Ianniruberto

Department of Chemical, Materials, and Production Engineering
Federico II University, Napoli (Italy)

Existing nonlinear rheological data of unentangled polymer melts indicate unexpected features, including a significant viscosity thinning in both steady shear¹ and steady uniaxial elongational² flows, which are incompatible with existing theories based on the Rouse model, even when accounting for the finite extensibility of the chains^{2,3}. Kuhn-segment orientation-induced friction reduction is confirmed to be the missing ingredient needed to describe the observed behavior, similarly to what previously found in entangled polymers⁴. Recent data on semi-dilute unentangled solutions also indicate the importance of orientation-induced friction reduction, but the effect is partially mitigated by a decrease of hydrodynamic interactions due to stretch-induced chain unravelling in fast flows⁵.

References

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. Ianniruberto, G.; Masubuchi, Y.; Marrucci, G. *Macromolecules* 2020, **53**, 13, 5023–5033
5. Costanzo, S.; Ianniello, V.; Pasquino, R.; Grizzuti, N.; Ianniruberto, G.; Marrucci, G. *Annual European Rheology Conference (AERC)*, Seville, April 2022.

Advances in rheology and polymer processing: A modeling and simulation point of view

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Polymer processing involves the shaping of polymer melts in various operations, such as extrusion, flow through dies, injection molding, wire coating, calendaring, fiber spinning, film blowing, blow molding, etc. The numerical simulation of these processes requires the solution of the conservation equations of mass, momentum, and energy, together with constitutive equations that adequately describe the rheology of the polymer melts.

In many cases, good shear viscosity data are sufficient to simulate well some processes, e.g. calendaring, wire coating, extrusion. In other processes where elongation is important, viscoelasticity plays a major role and requires modeling with sophisticated constitutive equations able to describe the viscoelastic character of the polymer in many different types of deformation. Such processes include flow through abrupt geometries, fiber spinning, film blowing, etc.

In the latter case, integral constitutive equations of the K-BKZ type have shown promise in: (i) fitting rheological data for the polymers, (ii) modeling polymer processing with strong shear and elongational components. Examples will be given for flows of polyethylene melts through extrusion dies, and also in fiber spinning, film blowing, film casting, and coating flows.

Towards miniaturization: how does confinement affect the break-up and coalescence of droplets in shear flow?

Paula Moldenaers

*Soft Matter Rheology and Technology, Department of Chemical Engineering, KU Leuven,
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For many years, polymer blending has been recognized as a method to generate materials with improved properties. When recycling polymers, the resulting morphology is also often multiphasic. The properties of these polymer blends are highly dependent on the flow-induced phase morphology. The bulk dynamics of immiscible blends during flow is relatively well understood, especially when the system consists of Newtonian components. Stimulated by the trend towards miniaturization, studies have recently focused on flow of immiscible blends in confined geometries. In that case, the morphology development is not only affected by the material properties and the flow type, but also by the degree of confinement.

In this presentation we discuss the morphological changes in dilute, immiscible two-phase blends in confined shear flow. Droplet break-up and droplet coalescence are investigated systematically for a range of viscosity ratios, where the droplets are visualized in a counter rotating shear flow cell equipped with a microscope. It was observed that geometrical confinement promotes droplet break-up when the viscosity ratio is above 1, which implies that the critical capillary number for break-up decreases. At viscosity ratios around one, confinement does not affect the conditions for droplet break-up whereas the critical capillary number increases with increasing confinement at viscosity ratios below 1, indicating that confined droplets are stabilized by the presence of the walls. Numerical simulations, using a boundary-integral method, in collaboration with TUE, reproduce and elucidate these findings.

For coalescence, on the other hand, the effects of confinement are qualitatively similar for all viscosity ratios; confinement decreases the coalescence angles and renders coalescence feasible at higher capillary numbers and initial offsets. Moreover, confinement induces a lower initial offset boundary, below which the approaching droplets reverse flow direction without coalescence. However, the range of conditions for which coalescence occurs decreases with increasing viscosity ratio. The results are supplemented with finite element numerical simulations in 2D to explain the observations.

REGULAR TALKS

Spinning a yarn of the molecular rheology of natural silk spinning: Sticky reptation in extensional flow

Charley Schaefer and Tom C.B. McLeish

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The rheologically-triggered transition, from semi-dilute protein solution to ordered fibre of natural silk, motivates an examination of the remarkable, and evolved, system of its molecular rheology. Polymer persistence, entanglement structure and electrostatics all combine with the nano-rheologically structured spinning duct of silk-worms, and the flow history of the spinning process, to create a sensitive flow-induced trigger for fibre formation.

A theoretical and computational study of minimal models for silk protein solutions [1, 2] demonstrates immediately that the usual approach of considering the ensemble-averaged conformational properties of the chains, while successful in understanding the rheology in start-up extensional flow of ordinary entangled polymers, is strongly violated in a number of other cases. These include the minimal model for silk solutions: associating (sticky) polymers in extensional flow (as well as linear polymers in shear and entangled ring polymers). Here, we develop coarse-grained simulations solve the conformational Brownian dynamics of entangled and unentangled sticky polymers, while the strain-dependent opening and closing of intermolecular associations are treated using a kinetic Monte Carlo algorithm. In the linear flow regime, we show through simulation and scaling arguments that the network weakens the dependence of the sticky-Rouse diffusivity on the sticker lifetime from the usual -1 power-law relation to a -4/5 power.

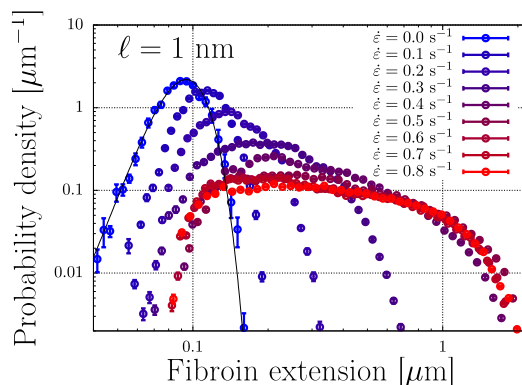


Figure 1. The distribution of fibroin stretch as a function of extensional flow rate develops a power-law tail for rates above a critical rate lower than the rate for stretch-divergence.

In the non-linear flow regime, we find a large dispersity of chain conformations of both sticky and non-sticky linear polymers in shear flow. We also confirm the onset of an emergent (non-Gaussian) power-law tail of the stretch distribution of sticky polymers in extensional flow below the stretch transition, suggesting a highly energy-efficient route to nucleation of solid fibers.

References

- [1] Schaefer, Charley, Peter R. Laity, Chris Holland, and Tom C. B. McLeish, ‘Silk Protein Solution: A Natural Example of Sticky Reptation’, *Macromolecules*, **53** 2669–2676 (2020)
- [2] Charley Shaefer and Tom C.B. McLeish, ‘Power Law Stretching of Associating Polymers in Steady-State Extensional Flow.’ *Phys. Rev. Lett.* **126** 057801 (2021)
- [3] C. Schaefer, P., Laity, C. Holland and T.C.B. McLeish, ‘Stretching of *Bombyx mori* Silk Protein in Flow,’ *Molecules* **26**, 1663 (2021)

Microstructural changes of concentrated Newtonian non-Brownian suspensions under oscillatory shear originating the failure of Cox-Merz rule

Claudia Carotenuto and **Mario Minale**

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Real Casa dell'Annunziata, via Roma 29, Aversa (CE) – Italy*

In a recent paper Carotenuto et al. (Rheol Acta 2021, 60, 309) showed that the complex viscosity of a Newtonian non-Brownian suspension is smaller than the steady shear one, whatever the imposed strain amplitude. Oscillatory shear is known to be capable of altering the microstructure of a concentrated suspensions through a shear induced particle diffusion mechanism. This mechanism needs time to show its effect and cannot be invoked to explain the observed mismatch between the steady shear and the complex viscosity, since the latter is typically calculated after maximum two or three cycles of oscillation. Moreover, in the limit of vanishing strain amplitudes the oscillatory shear should not alter the suspension microstructure and thus the complex viscosity should be equal to the steady shear one. The same should hold in the limit of very large strain amplitudes, where the oscillatory shear is equivalent to consecutive steady flow reversal that should regenerate the steady microstructure after each cycle. In these two limits the Cox-Merz rule should then hold.

With a combination of approaches exploiting the Lissajous-Bowditch plots, the Fourier transform rheology and the Sequence of Physical Processes, we investigate the microstructure changes induced by the sinusoidal flow in the first cycle of oscillation, so to limit the effect of diffusion mechanisms. We follow the microstructure evolution with the progress of the oscillations by investigating also the second and ninth cycle. The results obtained from the different analyses are in agreement with the microstructure rearranging mechanisms proposed by Carotenuto et al.. At small amplitudes, the oscillatory shear rotates couples of touching particles towards the flow direction, at medium amplitudes it breaks particle clusters and at very large amplitudes it reshuffles and reorients all the particles of the suspension. We also show that the vast majority of the microstructure rearrangement takes place soon after the flow inversion of the first cycle, while before it the microstructure is not altered. This allows us to suggest a procedure to “recover” the Cox-Merz rule validity: a single cycle of oscillation must be imposed and the stress response of the sole first quarter of oscillation must be analysed.

Ring polymer rheology and the limits of experimentation

Thanasis Athanasiou,^{1,2} Samruddhi Kamble,¹ Daniele Parisi,^{1,2} Taihuyn Chang,³ Jürgen Allgaier,⁴
Dieter Richter,⁴ **Dimitris Vlassopoulos**^{1,2}

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It is known that the absence of free imparts unique properties in polymers. Indeed, at high molar masses linear and branched polymers exhibit at rubbery plateau in their linear viscoelastic spectrum at intermediate frequencies, whereas ring polymers do not. The loopy character of rings also affects their nonlinear rheology, whereas blending of rings with linear chains has been shown to yield network reinforcement. These findings suggest that rings can be used as rheology modifiers. An interesting challenge is to understand the entangled state of rings and the role of molar mass. To this end, we combine well-characterized ring polymers of high molar mass with conventional and high-frequency piezo-rheometry to investigate their linear viscoelastic response. We show that the limits of experimental abilities are reached

and, using information from blending experiments, we propose that rheology is a very sensitive indicator of sample quality. We also present measurements of nonlinear shear rheology and normal stresses of rings and compare them against the respective linear data. Despite limitations, the results confirm the important role of loops in polymer rheology.

Non-linear-viscoelasticity characteristics of the gelation process

David Kogan and **Moshe Gottlieb**

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For quite a few decades the Winter-Chambon analysis [1] of the linear viscoelastic manifestation of the transition from liquid to solid-like gel has been successfully applied to a diversity of chemical and physical polymer networks [1,2]. Non-linear rheology and particularly large amplitude oscillatory shear (LAOS) has gained considerable attention in the last decade [3]. Analyses based on Fourier Transform rheology (FT-Rheology), Chebyshev polynomial expansion, and Lissajous plots have been suggested as means of characterizing LAOS behavior in different polymeric systems. Yet, little attention has been devoted to the non-linear behavior of crosslinked systems and more specifically, the evolution of non-linear rheological properties at the different stages of the crosslinking process. The question we wish to address is whether new insight into the gelation process and the ensuing structure of the polymeric networks may be gained by employing LAOS analysis.

For this purpose we have carried out LAOS measurements on chemically and physically crosslinked poly(vinyl alcohol) hydrogels (PVA). More specifically, two types of hydrogels have been studied: PVA networks formed by chemical crosslinking with glutaraldehyde and networks formed by freeze-thaw cycles. Reaction induced evolution of viscoelasticity during gelation of semi-dilute poly (vinyl alcohol) (PVA) in aqueous dispersions was studied through rheological measurements in the linear and non-linear domains. These measurements are contrasted with the properties of the physical gels formed by the freeze/thaw cycles. The work primarily focuses on the characteristics of the LAOS behavior near the gel point.

References

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3. Hyun, K. et al., “A review of nonlinear oscillatory shear tests: Analysis and application of large amplitude oscillatory shear (LAOS)” *Prog. Polym. Sci.* 36, 1697–1753 (2011).

Nonlinear shear rheology of nearly unentangled H-polymer melts and solutions

Salvatore Costanzo and Vincenzo Ianniello

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We investigate the linear and nonlinear shear rheology of a marginally entangled H-polymer melt and two solutions made by diluting high molecular weight H-polymers in linear oligomer. In order to approach a nearly unentangled state, dilution is conducted at volume fractions such that the two solutions attain a similar number of entanglements of the melt. Start-up shear experiments demonstrate that the nonlinear behaviour of the H-polymer melt is analogous to that of a linear melt with comparable span chain length. Concerning solutions, the increase of chain elasticity in fast flows, coupled with a lesser role of monomeric friction reduction, allows to attain strong stretch in start-up shear tests. As a result, transient strain hardening occurs. Furthermore, the viscosity thinning of solutions is strongly reduced.

Rheology of mature fine tailings

Jourdain Piette, Aref Abbasi Moud, and **Savvas G. Hatzikiriakos**

¹ *Department of Chemical and Biological Engineering, The University of British Columbia, Vancouver, British Columbia V6T 1Z3, Canada*

Oil sands tailings are a mixture of water, sand, clay, residual bitumen and lighter hydrocarbons, inorganic salts and water-soluble organic compounds that remain after extraction of bitumen from oil sands. These tailings are stored in basins called tailings ponds, which allow the solids to settle. The sand component of tailings settles out quickly, leaving the clay to form fluid fine suspensions. Over the years, the fine solids also settle to form a suspension called mature fine tailings (MFT). Processing and handling of the MFTs for environmental reasons (land reclamation) require a good understanding of their rheology. In this work the rheological characteristics of mature fine tailings (MFTs) were examined in both the linear and non-linear viscoelastic regimes. MFT samples exhibited thixotropic behaviour as well as apparent slip, which was suppressed by using sandpaper of grit 80 (200 m) at the wall of the parallel-plate geometry. The real yield stress of MFT with shear thinning behaviour was retrieved after fitting a Herschel-Bulkley equation. Creep and oscillatory shear tests are also used to verify the yield stress measurement. The yield stress of two MFT suspensions possessing similar volume fractions was found to be similar, however, a kaolinite suspension (formulated to mimic/match the MFT rheology) showed more shear thinning, and less thixotropy. The presence of bitumen remains in the MFTs (up to 2 wt%) suppressed to a large extent the apparent slip due to the immobilization of the particles at the interface. Finally, the effect of temperature on MFT rheology was studied in detail over the range of 0°C to 50°C showing a minimum viscosity and minimum yield stress at about 20°C (nonmonotonic increase with increase of temperature).

Rheology of dilute polydisperse bubble suspensions

Stamatina Mitrou, Simona Migliozi, Panagiota Angeli and Luca Mazzei

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Bubble suspensions are ubiquitous in a vast range of industrial applications, from the manufacturing of pharmaceuticals and cosmetics to the production of processed food. In all these contexts, the presence of bubbles can induce severe changes on the final texture and flowability of the products, thus highlighting the need for fundamental investigations on the rheology of these systems. This work seeks to examine the rheology of dilute polydisperse bubble suspensions in Newtonian media by experimentally investigating their steady-shear viscosity. Owing to their Newtonian behaviour and wide use in the pharmaceutical industry, a mixture of a viscous mineral oil and 28% w/w span 80 (surfactant) (4.2 Pa·s) was chosen as the ambient fluid for this investigation. To produce the bubbles, we implemented a custom-made aeration device, equipped with a propeller with attached aeration plates. This device provided simultaneous aeration and mixing, allowing us to achieve bubble volume fractions up to 21%. After the aeration, the suspensions were continuously mixed with a high-shear mixer to achieve smaller bubble dimensions, thus improving the stability of the mixture for the rheological measurements. For each sample prepared, a complete analysis of the bubble size distribution was carried out through optical microscopy followed by image analysis. We found that our suspensions were polydisperse with bubble sizes following the gamma distribution between 10 µm and 130 µm. To calculate a volume-weighted capillary number ($\langle Ca \rangle$) we employed the De Brouckere mean diameter (d_{43}) of the bubbles, which was found equal to 60 µm. The rheological properties of the bubble suspensions were investigated via steady-shear tests, during which we observed a double

power-law decay of the relative viscosity at capillary numbers between 0.01 and 1. For monodispersed bubble suspensions it has been proved that for very low and very high Ca the relative viscosity remains constant, while at Ca around 1 a steep shear-thinning behaviour is observed (Llewellyn et al., 2002a, Mader et al., 2013). Our results showed that the second decay of viscosity can be attributed to bubble deformation. When the bubble sizes follow the gamma distribution, the polydisperse suspension can be regarded as a monodisperse with average bubble diameter equal to d_{43} . For the effect of polydispersity to become apparent, the total bubble volume fraction should be divided between very small and very large bubbles. In this case, the presence of different bubble sizes generates different relaxation times, resulting into a more spread shear-thinning behaviour, which occurs over a range of capillary numbers spanning from 0.01 to 10. The first decay of viscosity remains an issue, which we will investigate further through rheo-optical experiments.

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Measurement of both normal stress differences using two partitions and piezoelectric sensor

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Nonlinear rheometry of viscoelastic materials such as polymer melts and solutions is technically demanding due to the intervention of edge fracture instabilities. By means of a partitioned plate fixture, i.e., an inner plate connected to the transducer and an external corona fixed on rheometer's chassis, one can significantly delay or even eliminate edge fracture in the inner measuring geometry. This provides the means to measure the shear stress over a range of shear rates. However, the presence of the partition makes the normal force measurement apparent, and to extract the first and second normal stress differences, two different geometries and/or loadings are needed. To bypass this cumbersome approach, which is also prone to errors, it has been proposed to use two partitions, the so-called CPP3 geometry. Earlier attempts were promising but measurements were too involved and with limited temperature control. In this work we propose a new method to measure the normal forces based on CPP3. While the outer corona mitigates edge fracture artifacts, the inner corona serves as a second fixture to measure the normal forces generated at shear start-up experiment. A piezoelectric sensor is coaxially mounted on the inner partition and the entire tool fit onto the rheometer's temperature control oven. The stiffness of the piezoelectric sensor rules out any force-rebalance complexities while its fast response provides also data in the transient regime. We discuss the design and implementation of this simple, robust tool and present some preliminary results demonstrating the proof of concept by ensuring the two normal stress differences in entangled polymer solutions and melts.

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S-PAL: A stabilized finite element formulation for computing viscoplastic flows

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Ideal viscoplastic models present an inherent discontinuity at the yielded/unyielded interface, which poses great numerical difficulties. In this work, the recently proposed method for the solution of viscoplastic flows, the Penalized Augmented Lagrangian (PAL) method [1] is coupled with a new projection-based finite element formulation that allows for equal order interpolants in all variables. The accuracy of the new finite element formulation is assessed by comparing its numerical results to those of the literature in three problems: (a) the buoyancy-driven bubble rise through a viscoplastic medium, (b) the steady-state lid-driven cavity and its transient counterpart, and (c) the transient gas-assisted displacement of a viscoplastic material in straight and corrugated tubes. The method presents increased numerical stability and reduced computational cost without hindering the accuracy of the solution. By changing the solution procedure, we are able to obtain solutions that are as accurate as those obtained with the Augmented Lagrangian AL method. In addition, we show that the optimal value of the penalty parameter is correlated with the mesh and the critical dimensionless numbers that correspond in each problem.

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A monophasic blood flow model for accurate prediction of wall shear stresses in the microcirculation

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Accurate simulation of 1D blood flow in microtubes has been made possible by the usage of biphasic models that account for the existence of a cell-free plasma layer adjacent to the walls [1-3]. In this work, we present an application-oriented approach by developing a monophasic steady-state model that retains certain non-Newtonian rheological characteristics of blood while replacing the cell-free layer with a slip condition on the tube walls. Understandably, the purpose of this formulation is not to reproduce with complete accuracy the velocity profile of blood in microvessels, but rather to allow for quicker and equally accurate (when compared to biphasic models) calculation of physiologically important quantities, such as the shear stress on vessel walls [4]. Our objective is achieved through the construction of a suitable explicit relationship for the slip parameter, which is calibrated via regression on the biphasic model results. The procedure of model development is complimented by simulations of steady-state blood flow within realistic microvascular network structures. Further investigation reveals that the monophasic model is able to closely follow the wall shear stress predictions of a biphasic model, exhibiting deviations below 2% of the expected value when vessel radii and discharge hematocrits range between 10-75 μm and 0.2-0.7 respectively. Vessel network simulations prove the significant reduction in computational time -almost by an order of

magnitude- offered by the utilization of the monophasic model. Our approach is valid for a wide range of physiological conditions within the human microcirculation. The model performance is extremely satisfactory, to the point that we are very optimistic of its ability to extrapolate beyond the aforementioned ranges. In any case, we believe that the modeling procedure is sufficiently streamlined, so that one can easily work on expanding the model's applicability range, which may be necessary when trying to account for pathological cases.

Acknowledgements

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Blood viscosity in passive microchannel flows: effects of erythrocyte deformability, aggregation and haematocrit

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Passive microchannel flow is an alternative approach to the technology-intense pressure driven setups used in blood diagnostics. The main drawback in the passive (surface tension driven) flow is the uncertainty introduced in the flow behaviour by the fluid properties, mainly viscosity, affecting the performance of such devices. In the case of blood, the donor to donor variations and the alterations in the fluid physiology due to pathologies, can intensify the aforementioned uncertainties. In this work, the effects of erythrocyte deformability, aggregation and haematocrit, were examined in the passive flow of a converging, and of rectangular cross section, microchannel. The flow was assessed using micro-Particle Image Velocimetry (μ PIV) based, and tracking techniques. An analytical solution for the meniscus velocity was utilized to estimate the viscosity of the fluid samples using a power law viscosity approximation. The increasing sample viscosity and the reduced erythrocyte deformability affected the mean velocity of blood as expected. The erythrocyte aggregation phenomenon affected the local and bulk velocity characteristics in a non-intuitive manner. Very high shear rates were observed in the early stages of the flow, persisting sufficiently strong until the flow reaches the end of the channel. The predicted viscosity from the microchannel flow data confirmed the effect of the high shearing conditions in the flow and proved efficient for the estimation of the high-shear viscosity of blood.

Acoustic interrogation of coated microbubbles in a wall restricted flow: the compression only and microstreaming effects

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In the present study we investigate the dynamic response of coated microbubbles to acoustic disturbances in a presence of a wall and we mainly focus on the compression only behaviour of lipid shelled microbubbles (contrast agents) that has been reported in many experiments¹, as well as the microstreaming effect that has been mainly studied theoretically and experimentally for uncoated bubbles^{2,3}. The Galerkin Finite Element Methodology is employed for the spatial discretization of the flow domain and the continuity and Navier-Stokes equations are solved for the liquid. The coating of the bubble is assumed to have constant rheological properties and is described as a viscoelastic shell with bending resistance while the dilatational and shear viscosity of the membrane are treated as different. Numerical simulations reveal that lipid shells are possible to develop a compression only behaviour (Figs. 3a,b) during which they oscillate around compressed buckled shapes that belong to static branches that are energetically favoured. An initially prestressed shell facilitates the onset of buckling at relatively small acoustic disturbances, whereas low values of the shear viscosity compared to dilatational viscosity facilitate parametric onset of shape modes that characterize these static solutions. The phase diagrams, constructed based on the stability analysis for an inviscid and unbounded flow, are enriched with the numerical simulations in order to incorporate the effect of a nearby wall and a parametric study is conducted to define the conditions for the onset of the phenomenon. Depending on the sound amplitude as well as the compressed buckled shape, the microbubble is seen to, move towards the wall and eventually get trapped, move away from the wall for asymmetric buckled shapes and intense compression only behaviour, or collapse above a certain amplitude threshold. The streamline flow pattern is also examined, for both uncoated and coated bubbles (Fig. 3c) to investigate the conditions and the mechanism for the onset of microstreaming and a parametric study is conducted in terms of the shell properties, sound disturbance and liquid viscosity.

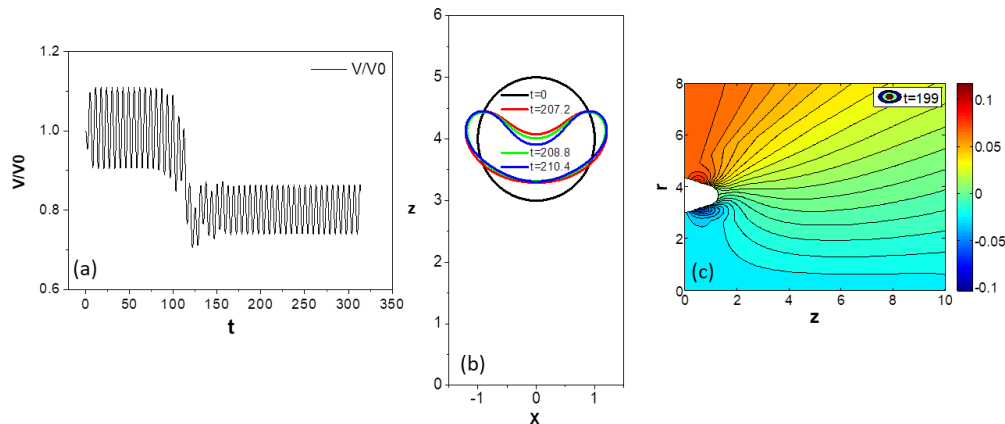


Figure 1: (a,b) Compression only effect for a lipid shell and (c) snapshot of the stream-lines during the compression only effect.

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A multiphase model of vascular smooth muscle cell

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Vascular Smooth Muscle Cells (VSMCs), one of the primary components of the arterial walls, change their dimensions, structure, and morphology in response to mechanical stimuli [1]. Through contraction and relaxation, vascular SMCs regulate the local blood flow and control the vascular tone. Thus, to investigate in-depth, the behaviour of the vascular walls, it is essential to know the mechanical properties of SMC in the dilated and extracted state. VSMCs are splined-shaped and their intracellular space encompasses the nucleus, the cytoskeletal as well as smaller organelles, and filaments, which run mostly parallel to their major axis and determine the mechanical properties of the cell [2]. In the present study, we examine the dynamics of the cell under compression and extension and identify the mechanical properties of the cytoplasm. To this end, we have developed a three-dimensional multiphase model that incorporates the structural dynamics and the interactions between the main subcomponents of the SMC; including the nucleus, plasma membrane, and cytoplasm. More specifically, the nucleus is treated as a hyperelastic solid, whereas the plasma membrane that surrounds the cell is represented as a thin, almost rigid, layer. Based on the structure of the cytoskeleton, the cytoplasm is modelled as a fibrous poroelastic medium. The cytoplasm parameters, including the elastic and shear moduli in the directions parallel and transverse to the filament orientation, are estimated by fitting the results of the simulation with previous experimental and numerical studies.

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Role of the hydrophobic phase on interfacial phenomena of surfactants, proteins, and particles at fluid interfaces

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The formation of viscoelastic networks at fluid interfaces by adsorption layers is essential in many industries, scientific disciplines, and biological processes. However, the effect of the oil phase on the structural transitions of proteins, adsorption of surfactants and particles, subsequent network formation, and layer strength at fluid interfaces has received little attention in interfacial experiments and emulsion design. This has been the cause for significant inconsistencies in the scientific literature, as experiments were often performed at arbitrary oils, which impeded the reproducibility and comparability as well as hampers the pathway to a generic description. Here, we summarize the effect of the oil phase on the adsorption,

assembly, and interfacial rheology of surfactants, proteins, and particles at fluid interfaces and the resulting influence on emulsions [1-6]. Furthermore, we provide experimental guidelines for using oils in interfacial experiments, aiming to harmonize results and protocols in interfacial science.

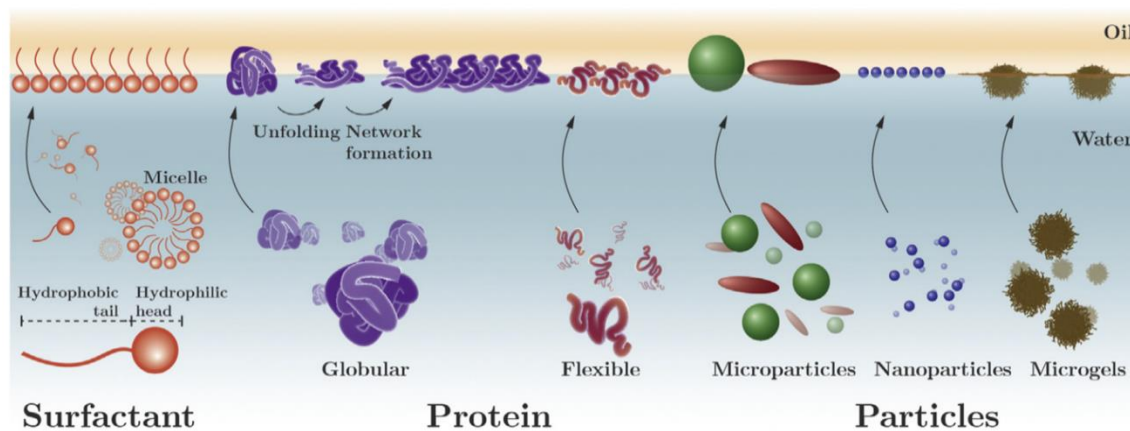


Figure 1. The adsorption of surfactants, proteins (globular and flexible), and particles (micro- and nano-sized and soft particles) to fluid interfaces [6].

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Effects of surface-active nanoparticles and surfactants on the migration of drops in nanochannels

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Surfactants and nanoparticles can stabilize oil-water interfaces, but the stabilization mechanism is different in each case. While surfactants lead to a reduction in interfacial tension (IFT),^{1,2} nanoparticles do not change the IFT but reduce the oil-water interfacial area. The present work is focused on a detailed investigation of the combined effects of surfactants and nanoparticles at the interface of drops, and on how observed behavior is than when either surfactants or nanoparticles are present on their own. Applications cover phenomena in environmental remediation of soil contaminated with organic compounds, enhanced recovery of hydrocarbons with chemical flooding,^{3,5} separations, and drug delivery.^{6,7} Here, coarse grained computations with the dissipative particle dynamics methodology (DPD) were employed to observe the migration of sessile oil drops in water and of drops that extend from one wall to the other in a nanochannel. Janus nanoparticles, where one side is hydrophobic and the other side is hydrophilic, and octaethylene glycol monododecyl ether (C12E8) were used. The oil phase was hexadecane. For the sessile drops, a plane Couette flow field was employed to control the shear in the nanochannel. It was found that surfactants enhance drop displacement, but nanoparticles tended to impede this displacement. The transport of momentum from the water to the oil phase was enhanced with surfactants, but the friction induced by the

motion of nanoparticles moving to the drop contact line with the wall decreased oil displacement. When surfactants were added to the drop along with nanoparticles, the displacement increased. For the case of drops extending from one wall to the other, a Poiseuille flow field was employed. Interfacial instabilities would grow in the form of finger instabilities when surfactant only was present, but they would be impeded when nanoparticles were present. The presentation will discuss the computational methodology and its validation, the mechanism of stabilizing the oil-water interface with nanoparticles and surfactants, and the implications for tuning oil-water interfacial behavior.

Acknowledgments

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Novel instabilities in immiscible multilayer viscous shear flows in the presence of interfacial slip

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Single phase Couette flows are known to be linearly stable at all Reynolds numbers. When two immiscible viscous stratified fluids are sheared in a channel an interfacial instability is possible at all non-zero Reynolds numbers. Typically, a no-slip condition is appropriate at fluid-fluid interfaces and the linear and nonlinear stability of such configurations (including direct numerical simulations) has been studied extensively [1].

It has been observed in experiments [2] on coextruded multilayers of polymer-polymer systems, that interfacial slip is present and responsible for unexpected increased flow-rate measurements. Molecular dynamics simulations have also demonstrated the presence of slip at liquid-liquid interfaces for both Couette and pressure-driven flows. The MD simulations also demonstrated that a Navier-slip law is very successful in describing the data.

The present work is a theoretical study of the effects of Navier slip at liquid-liquid interfaces. Guided by experiments we concentrate on Newtonian flows and undertake a comprehensive study of the linear and nonlinear stability of such systems. To fix matters we consider two-fluid Couette flows. In the presence of slip the basic flow undergoes a velocity jump at the interface that depends on the slip length. The mathematical models are viscous analogues of the classical Kelvin-Helmholtz instability present in co-flowing ideal flows. Asymptotic solutions are constructed for large slip and short or long wave disturbances to isolate the novel instability mechanisms. In the case of short waves (with surface tension absent) it is shown analytically that the growth rate tends to a non-zero constant that depends on parameters, in contrast to the slipless case where the growth rate decays to zero inversely proportionally to the large wave number. This scenario persists for finite values of the slip length. The new instabilities are quantified via computations of the full eigenvalue problem. Time permitting, a nonlinear theory when one of the layers is thin will be presented; the dynamics are described by a novel integro-differential evolution equation and the role of slip will be reported from numerical simulations.

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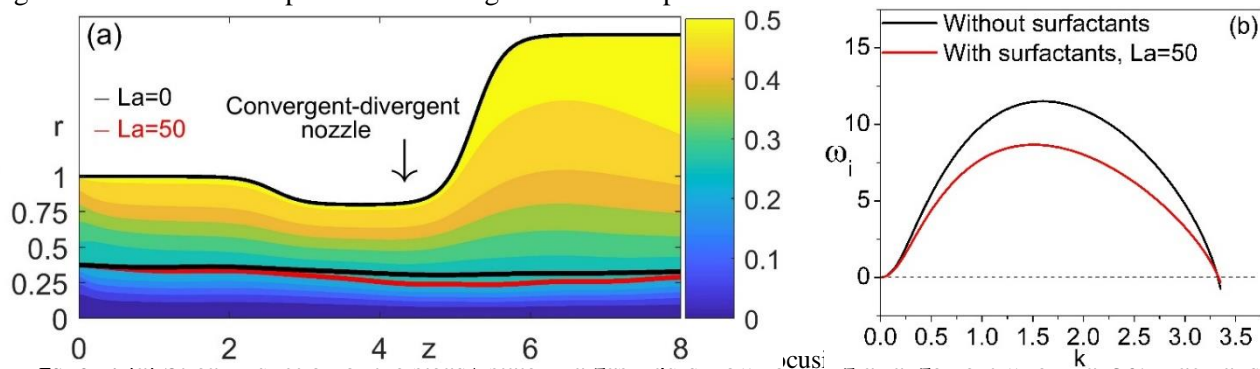
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Steady state and dynamic simulations of axisymmetric gas-liquid flow focusing arrangement in the presence of surfactants

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Encapsulated bubbles have received significant attention due to increasing number of applications especially in targeted drug delivery and medical imaging. Their behavior in the vascular bed is controlled by the viscoelastic properties of the coating, which usually consists of surfactants or polymers. Microfluidic devices have emerged as a robust tool for the formation of microbubbles coated with surfactants, because they ensure a highly controlled size and well-defined rheological properties¹. In this study, we investigate the axisymmetric gas-liquid flow with liquid focusing in the presence of surfactants. The Navier-Stokes and the mass transport equations with the dynamic and kinematic conditions are discretized with the finite element method, while the mesh is generated with a spine transformation. Steady state asymptotic analysis and numerical simulations reveal that the bulk concentration of the surfactant exhibits almost no variations within an $O(\text{Pe}^{-1})$ boundary layer formed across the interface, as we raise the characteristic velocity. Parametric analysis shows that as the ratio of the annulus to core viscosity increases or as the surface surfactant concentration increases, the interface approaches the axis of symmetry. Spatial instabilities are captured on the interface in the steady base flow, when we consider a flow focusing geometry, Fig 1(a), that are amplified in the presence of surfactants, i.e. with increasing Langmuir number, La . Linear stability analysis is performed for a wide parameter range and it is found that in contrast with steady state Marangoni stresses tend to lower the growth rate, Fig. 1(b), while the opposite happens when we increase the viscosity ratio. Short wave-length instabilities are captured as the viscosity ratio increases or as the interface moves closer to the axis of symmetry. The emerging instabilities can change from convective to absolute by increasing the surface tension. Direct numerical simulations capture the onset of long or shorter wave-length instabilities that lead to pinching. A more sophisticated representation of the interface and mesh generation with the elliptic method will give a detailed picture of the microbubble formation mechanism.



red lines represent the position of the interface in the absence and presence of surfactants. (b) Growth rate curve. $R=89$, $M=82$, $Q_2/Q_1=1$, $We=8.52 \cdot 10^{-4}$, $Ca=1.6 \cdot 10^{-4}$, $\beta=0.624$, $Pe=5787$.

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A parametric study of dynamics of liquid lens spreading over a viscoplastic liquid substrate

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The scope of the present study is the detailed investigation of the non-linear transient dynamics of a liquid lens spreading over a viscoplastic fluid layer. The viscoplastic behaviour of the liquid subphase is accounted for by considering a liquid governed by the continuous Herschel-Bulkley constitutive model based on the Papanastasiou regularization. The governing flow equations are solved numerically using our newly developed solver, rheoMultiFluidInterFoam, which is based on a finite volume method and the volume of fluid (VOF) method. The multiphase nature of the system is considered by utilising a continuum surface force model. The interface tension pairings between the different phases are handled by using the interfacial tension coefficient decomposition method. The present computational model is successfully validated through comparisons with existing analytical and numerical solutions in the two- and three-phase flows involving Newtonian and/or non-Newtonian fluids. The lens shape, the shape of the yield surfaces, the pressure, the velocity and stresses fields are determined for several values of the Bingham number in order to assess the impact of the rheological characteristics of the subphase on the droplet spreading. The effect of density and surface tension ratios between the three phases and the influence of the fluid layer depth are also examined. As the Bingham number is increased the lens spreading is significantly attenuated, reaching a different state from that expected in the pure Newtonian case. The lens continues to spread over the very viscous liquid which has become completely unyielded.

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Bubble rise in elastoviscoplastic materials

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The peculiar dynamics of bubbles rising in complex fluids has been studied extensively over the past few decades, starting with the pioneering work by Astarita and Apuzzo^[1]. They are frequently encountered in industrial operations, like polymer or cement processing, and their presence can lead to undesirable consequences like mechanical degradation of the final product or safety issues. To this end, we undertake a novel computational study to examine the buoyancy-driven rise of a bubble in a yield stress fluid that is characterized both by elasticity and yield stress. The Saramito Herschel-Bulkley model^[2] is used to model the rheological behavior of the material. The governing momentum and mass balance equations are solved numerically using the newly developed finite element method for free surfaces by Varchanis et al.^[3], namely PEGAFEM-V. Furthermore, we assume axial symmetry, and that the center-of-bubble volume remains at the origin of the coordinate system. An elliptic grid generation scheme is used to track the bubble-fluid interface^[4]. The results regarding the bubble shape and the terminal velocity are in agreement with recent experimental data by Lopez et al.^[5] and Pourzahedi et al.

^[6] for different bubble sizes and Carbopol solutions. We analyze thoroughly the shear and normal stresses acting along the bubble surface because they provide insights into the underlying physical mechanisms. For smaller bubbles, large normal stresses arise in the trailing edge of the bubble due to the presence of elasticity, thus bubbles attain an inverted tear drop shape. Also, the negative wake structure appears behind the bubble. However, for larger bubbles, inertia overcomes elasticity, and the bubble shape changes to that of an oblate ellipsoid or spherical cap. Moreover, we perform a parametric study varying the rheological properties of the material, i.e., the shear modulus and the consistency index. Finally, a comparison of bubble dynamics in elastoviscoplastic and purely viscoelastic materials is presented.

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Flow development of power-law fluids in tubes and channels

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The flow development of power-law fluids in long pipes and channels is studied by means of finite-element simulations. In addition to the standard development length, L_c , which is based on the development of the centreline velocity [1], the development length is also calculated as a function of the transverse coordinate, in order to determine the global development length, L_g [2-4]. We also define the stress development length, L_t , based on the evolution of the wall shear stress. Results have been obtained for values of the power-law exponent n ranging from 0.2 to 1.5 and for Reynolds numbers (Re) up to 1000. In pipes, centreline and global entrance lengths coincide for $n > 0.7$, i.e., the flow indeed develops more slowly at the symmetry axis. This is not the case, however, as the fluid becomes more shear thinning. Big differences are observed, which are more pronounced at low Re (Fig. 1a) The stress entrance length is smaller than the classical centreline entrance length except for $n < 0.4$ and $n > 1.45$. More dramatic are the differences in channel flow. For $n < 1$ (shear thinning), L_c is smaller than L_t and L_g (Fig. 1b). The differences are relatively reduced as Re and n are increased.

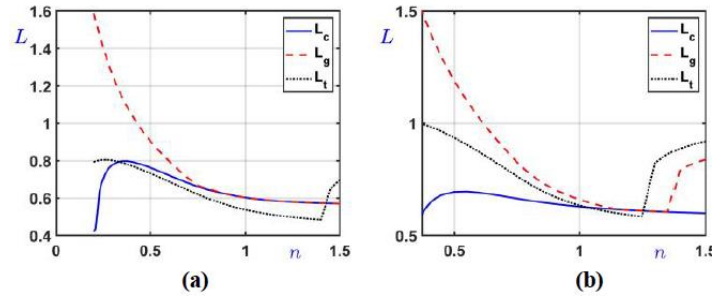


Figure 1: Centreline, global and stress development lengths at zero Reynolds numbers: (a) Pipe flow. (b) Channel flow.

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Study of dendronized polymers across different length scales and concentration regimes: State of the art and future perspectives

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Dendronized Polymers (denpols) belong to the general class of thick polymers comprising a linear backbone with grafted tree-like structures (dendrons). The dendritic side-chains give rise to the molecular thickness which can be tailored by altering the generation [1]. Recently, we investigated the conformational properties of these macromolecules in the dilute regime using scattering experiments and molecular dynamics simulations, to obtain their form factor and assess the role of increasing generation [2]. Denpols were found to behave akin to bottlebrushes at such low concentrations, however, in the melt they exhibited differences among concentrations G , especially for $G < 3$. The viscoelastic relaxation spectrum was found to bear signatures of dendron interpenetration and backbone motion [3]. For $G < 3$, the spectrum is distinct and was interpreted in view of the pertinent structural information, revealing that dendron interpenetration leads to a solid-like mode with modulus in the 10 MPa-100 MPa range which drives the system into the glassy regime. The interplay of dendron interdigitation and backfolding, which can be interrogated by combining rheometry and scattering, is believed to give rise to a non-monotonicity of the terminal relaxation time with increasing generation. Hence, denpols exhibit distinct rheology compared to other highly branched architectures such as bottlebrushes, dendrimers or hyperbranched polymers. Finally, in an attempt to better understand this complex class of materials we discuss our efforts to bridge the two regimes of interdigitation and backfolding by investigating concentrated solutions using both experimental methods as well as coarse-grained simulations.

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Extensions of Frenkel’s Model of Viscous Sintering

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Sintering (coalescence) of particles is frequently encountered in many industrial and natural processes. Frenkel’s model is based on the assumption that the driving force is surface tension resisted by viscous and, in some cases, viscoelastic forces. The original model was applicable for the start of the process for a pair of spheres. It was subsequently extended to completion (full coalescence). The basic assumption of extensional flow is retained from start to the end of the process. The model predicts neck growth as a function of time, using two independently measured parameters: viscosity and surface tension. Despite the simplification of an essentially 3D flow problem, the model was found to be in good agreement with experiments involving polymers, biomaterials and glasses. The time scales involved ranged from seconds to hours. Beyond the spherical geometry of the original model, an extension was made to a pair of cylinders and for square packing of an array of cylinders. Temperature dependence of viscosity has also been included. Recent work involved unequal doublets of spherical and cylindrical geometry. Determination of neck size is problematic, experimentally, for unequal size particles. Comparisons were made using other measures of coalescence such as particle circularity. Satisfactory agreement was obtained with experiments available in the open literature. Practical applications of the model include rotational molding of polymers, laser sintering, fused filament fabrication, coalescence of biomacromolecule-rich droplets and more.

***In situ* custom-made rheological setup for real-time mechanical characterization of crosslinking reactions**

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Recording the kinetics of hydrogels during the reaction process is a challenging research topic providing insightful information for the physicochemical and mechanical response of the system. Our research aims at introducing a new rheological setup for *in situ* real-time mechanical characterization of crosslinking reactions, presented in Besiri *et al.* (2020) [1]. The setup simulates the operating principle of a batch reactor. It consists of two parts creating an inner cavity, when these parts are mounted. The concept of the process is that ionic solution is supplied in the cavity and it comes on the top of the setup through microscale holes, where it diffuses into the polymer and the reaction begins. The alginate-Ca²⁺ system is used as the crosslinking network. Alginate, as a negatively charged long-chain polymer, reacts with Ca²⁺ cations, in aqueous solutions and forms hydrogels through ion crosslinking, following the “egg-box” model.

Our *in situ* method can successfully and continuously record the alginate-Ca²⁺ kinetics from the very beginning. The sol-gel transition, occurs in the first seconds of the process, can be detected. Oscillatory time sweep experiments at 1 rad/s angular frequency and 3% strain, in the linear viscoelastic region, record the evolution of the reaction. The storage, G' , and loss, G'' , moduli rapidly increase in the beginning of the process, due to the formation of the first ‘egg-box’ structures. As a long-term response, the moduli tend to

reach plateau values. This stage is called quasi-steady state, since the G' continues to increase, but with a slow rate comparing to the first stage of the process.

The present research efforts focus on the improvement of the setup to increase homogeneity of the ions into the polymer, as well as a better distribution of the gelling structure at the periphery of the parallel-plate geometry. Finally, with a mathematical equation, the reaction kinetics and the assessment of important parameters is described.

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Flame-patterns and diwhirls in elasto-inertial Taylor Couette flows*

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Taylor-Couette (TC) flow, the flow between two concentric cylinders with one or both of them rotating, has served as a paradigm for studying flow instabilities for almost 100 years since the seminal work of G.I.Taylor. Despite the simplicity of the geometry, in the case of viscoelastic TC flows, a variety of transitions, leading to the onset of Elasto-Inertial Turbulence (EIT), have been reported. A vortex merging and splitting transition (MST) has been reported for shear-thinning or moderately elastic fluids [1], whereas a chaotic state of strong radial inflow jets, often termed flame-pattern (FP), appears for fluids of higher elasticity [2]. A hysteretic behavior has also been reported characterized by stationary structures of strong inflow jets, called solitary vortex pairs or diwhirls (DW) [3].

We study the instabilities induced by Boger fluids with different elasticities ($El = 0.057 - 0.341$) in a TC flow with a rotating inner cylinder, both for ramp-up and ramp-down conditions in the range of $Re = 0 - 200$. Flow visualization experiments using mica flakes were conducted to produce spatiotemporal maps in order to identify the transitions. In low elasticity, the previously reported MST route to EIT is observed. In higher elasticity, the MST gives rise to FP and hysteretic DWs are observed during ramp-down. FPs become progressively more chaotic with increasing inertia, leading to EIT. The nature of the FP/DW instability and the route to EIT are elucidated using PIV measurements in selected Reynolds numbers.

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Network formation in carbon nanotube polymer-based nanocomposites during injection and compression molding

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Carbon nanotubes (CNTs) are nanofillers with high strength and effective electron transfer. Their anisotropic nature (rod-like geometry) enables the formation of randomly connected network in polymer-based matrix, which can be explored as mechanical reinforcement and/or conducting pathway in several technologies. However, the functionality as well as the end properties of such polymer-based CNT nanocomposites mainly depend on network formation and its configurations established in the melt state where various mechanisms are present (erosion, rupture, diffusion). It is obvious that melt processing techniques (first stage - mixing, extrusion, second stage - injection molding, compression molding), affect network differently and thus the final properties of the processed materials.

The present research studies the effect of melt processing techniques on network formation and its impact on the mechanical reinforcement of single-walled carbon nanotube (SWCNT)/high- and low-density polyethylene (LDPE and HDPE) nanocomposites. Melt mixing was used as the initial processing method, while injection and compression molding were used as the second step.

Plasma-etching coupled with electron microscopy as well as rheological analysis have shown that network is established from SWCNT bundles, which geometrically entangle at critical volume fraction of $\Phi_{v,crit} \approx 0,4\%$ in LDPE and HDPE nanocomposites regardless of the processing technique used. A profound difference in network configuration was observed for injection or compression molded samples, respectively. Above $\Phi_{v,crit}$, both processing techniques resulted in random network configuration (movement of bundle was constrained by neighboring unit). However, below $\Phi_{v,crit}$ (bundles may rotate freely about their center mass) the injection molding enabled the alignment of the bundles in the flow direction, while the use of compression molding resulted in random configuration. Furthermore, the reinforcing functionality of nanocomposites was evaluated by nanoindentation. The results confirmed the critical entanglement $\Phi_{v,crit}$ of SWCNT bundles (as determined by rheological analysis), which additionally contributed to mechanical reinforcement. Moreover, it was found that the processing techniques have no effect on the mechanical properties, despite the differences of network configuration below $\Phi_{v,crit}$.

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Thixotropic modelling of yield stress fluids

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Thixotropy is a characteristic behavior of many yield stress materials wherein, the material exhibits a time dependent shear-thinning behavior due to structural breakdown when sheared and may regain its original structure over time at rest. In this study, the thixotropic behavior of three commercially available stirred yogurts, Carbopol® 980 NF and 981 NF polymers is examined. The goal of the study is to examine the capability of various models to predict the thixotropic behavior of the test samples between different thixotropy tests. Thus, experimental data from hysteresis loop tests, i.e., applying shear rate ($\dot{\gamma}$) sweep up and down while recording shear stress (σ) response, is fitted with various thixotropic models having an equation of state and a rate equation. The test samples show a hysteresis loop due to differences in the rate of structural breakdown and buildup. The fitted model parameters are then used to predict the behavior of the test samples in thixotropy recovery tests, i.e., having multiple applied low and high shear stresses below and above the yield stress. Several experimental protocols for both hysteresis loop and thixotropy recovery test are considered to evaluate model fitting and predictions. Furthermore, creep tests are performed to obtain the yield stress range of the test samples.

A thermodynamically consistent, microscopically-based, model of the rheology of aggregating particles suspensions

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In this work we outline the development of a thermodynamically consistent, microscopically based, model for a suspension of aggregating particles, based on the Single Generator Bracket Formalism (SGBF) of NonEquilibrium Thermodynamics as developed by Beris and Edwards [1]. We show how the combination of an appropriate population balance-based description of the aggregating particle microstructure along with the use of the single generator bracket description of nonequilibrium thermodynamics, can lead effortlessly to the formulation of the model equations. Notable elements of the model are: a lognormal distribution for the aggregate size population, a population balance-based model of the aggregation process and a conformation tensor-based viscoelastic description of the elastic network of the particle aggregates. The resulting model is evaluated in steady and transient shear and elongational flows and shown to offer predictions that are consistent with observed rheological behavior of typical systems of aggregating particles. Additionally, an expression for the total entropy production is also provided that allows one to judge the thermodynamic consistency as well as to evaluate the importance between the various dissipative phenomena involved in given flow processes.

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Multi-scale simulation approach to morphology and microrheology of mixed surfactant-cosurfactant micellar solutions

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Liquid formulations based on anionic surfactants find numerous applications today in cosmetics, health, and personal-care products. In the absence of salt, surfactants in aqueous solutions organize into spherical or tiny rod-like micelles, and their zero-shear viscosity is close to that of water. Adding small amounts of salt alters the shape of micelles and increases their size resulting in what is known as wormlike micelles (WLMs). Their zero-shear viscosity increases by several orders of magnitude approaching a peak value beyond which adding more salt causes a decrease in the viscosity, and the fluid exhibits shear thinning and viscoelastic response.¹ These fluids are characterized by a complexity of interactions and present morphology and dynamics across a truly broad spectrum of characteristic length and time scales that renders their direct MD simulation a formidable task.

We present here a hierarchical approach combining a variety of computational tools (coarse-grained simulations reverse-mapped to all-atom ones,^{2,3} and subsequent mapping onto a Brownian Dynamics algorithm) which allows us to access length scales on the order of micrometers (i.e., commensurate with the contour length of the wormlike micelles under equilibrium conditions) and address micelles characterized by large mean aggregation numbers, up to 1000. Our emphasis is mostly on the impact of salt on the morphology of the micelles formed by anionic surfactants and their mixtures, using as a model system a mixture of sodium laureth sulfate (SLES) as the base surfactant.

Our simulations show that small spherical micelles are formed in salt-free conditions. By gradually increasing the salt concentration leads initially to the formation of small cylindrical micelles, which upon further addition of salt self-aggregate to form long wormlike micelles with several nanometers in size, in agreement with experimental observations.¹ The presence of co-surfactant mediates additional molecular interactions and further enhances the viscosity of the formulation. A mesoscopic Brownian Dynamics code parameterized on the findings of lower scale simulations is currently under development to address the linear- and non-linear rheology of the same solutions.

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Cage formation and dynamics in repulsive and attractive glasses probed by high frequency rheology

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The cage idea has been widely utilized in colloidal suspensions as a central microscopic concept to describe a number of phenomena related with glassy dynamics. Here we probe the evolution of cage formation and shear elasticity in colloidal suspensions approaching and well inside the glass regime. Emphasis is given in the short-time dynamics utilizing linear viscoelastic (LVE) measurements by means of conventional rheometers and a home-made high frequency (HF) piezo-rheometer [1] to probe the dynamic response in a broad range of volume fractions up to the very dense regime in proximity to RCP. We focus on the LVE spectra and on short times, where the caging effect is not so evident as the particles cannot fully explore their cage. This results to the virtual solid to liquid transition at elevated frequencies marked by the HF moduli crossover. On the other hand, caging becomes tighter as volume fraction increases and the in-cage rattling becomes more localized shifting the HF crossover to higher frequencies. The study of the dependence of the HF crossover properties (frequency and moduli) on volume fraction provides direct insights of the particle in-cage motion, and allows comparison with current theoretical models. We find that the above characteristic HF crossover properties exhibit two nearly exponential dependent volume fraction regimes. This experimentally robust finding is consistent with predictions of the microscopic nonlinear Langevin Equation dynamical theory (2) with highly accurate structural input (3). We further explore the effect of attractive interactions either via the addition of linear polymer chain depletant or by inducing via slight refractive index mismatch van der Waals attraction. Particle localization is now determined by both entropic caging and enthalpic bonding, altering the high frequency viscoelastic response of the system.

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Evaluation of the microrheological properties of blood cells using microfluidic methods

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Microfluidics has become a prominent field for studying blood microrheology and mechanical properties of blood cells - erythrocytes, leukocytes and platelets. This work reviews the recent developments in microfluidic technologies for *in vitro* tests of red blood cells (RBCs) deformability and RBC aggregation, leukocyte aggregation and adhesion, and platelet thrombus formation. The study summarizes the working principles and experimental results of key microfluidic platforms for RBC deformability, RBC aggregation, leukocyte aggregation and platelet coagulation and thrombus formation. The advantages and limitations of these techniques are examined and discussed. Results for RBCs aggregation and adhesion of leukocytes, as well as for thrombosis, their mutual influence observed in some pathological conditions are shown.

The developed devices and experimental systems are promising tools for the study of erythrocyte deformability and aggregation, as well as leukocyte adhesion and thrombus formation.

Acknowledgements

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Modelling of Polymer/Alumina Interfaces via Ab-initio Calculations and Machine-learned Molecular Dynamics Simulations

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The properties of polymeric nanostructured materials are typically determined by the presence of polymer/solid interfaces. Polymer chains in interfaces are characterized by a very broad range of characteristic time (from fs up to sec) and length (from Å up to several nm) scales [1]. The latter and the complex quantum mechanical interfacial interactions indicate that multiple spatiotemporal scales must be bridged. Here, we study such systems via a new hierarchical multi-stage simulation methodology, involving ab-initio calculations and atomistic simulations of polybutadiene (PB)/alumina interfacial systems. Initially, density functional theory (DFT) calculations of a single butadiene monomer adsorbed on alumina surface are performed. We sample the energy and configurations of the system via constraint DFT minimizations based on adsorption characteristics. In the second stage, a detailed (classical) atomistic force field is obtained for the butadiene/alumina interaction by machine learning (ML) algorithms using pairwise additive parametric functional forms, e.g. Lennard-Jones, to fit the DFT data [2]. The last stage of the proposed hierarchical simulation approach concerns the prediction of the properties of PB/Alumina interfaces at the atomic level, using the developed classical atomistic force field. We study the structure, conformations and dynamics of polymer chains as a function of distance from the alumina substrate.

Keywords: interfaces, MD, DFT

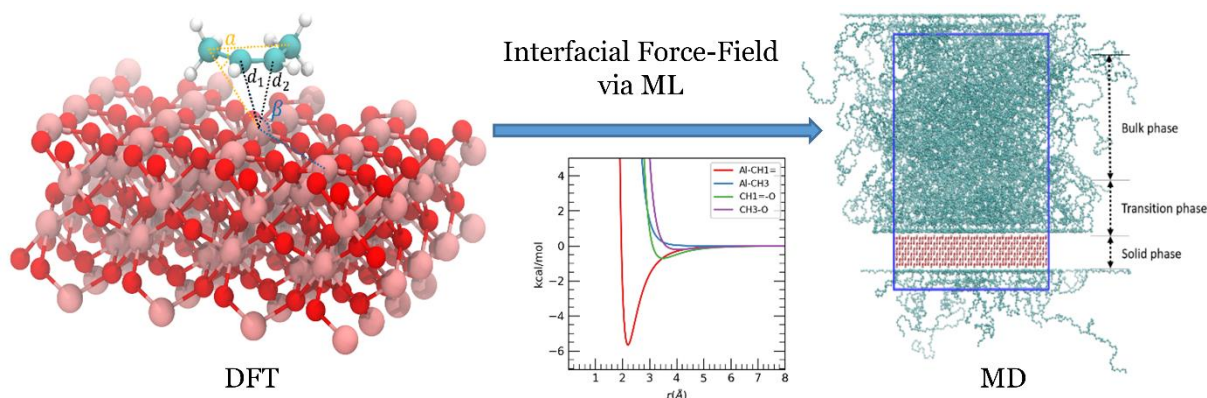


Figure 1. Schematic of the multi-scale methodology. Initially, distances d_1 , d_2 and angles α , β are constrained for many different values to sample the configurational space. We fit the DFT data by a ML algorithm and we obtain pairwise potentials that are applied in MD simulations. We calculate the gradient of properties within the transition phase.

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Exploring quenchant properties at the nanoscale – A molecular dynamics study

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Metal quenching is the heat treatment process where a component is heated up to 1100 K and then rapidly cooled to room temperature. The selection of new quenchants (e.g. Aqueous Polymer Solutions – APS and nanofluids) is primarily based on experimental observations, trial and error and empirical correlations, with a lack of understanding of the underlying physical heat transfer mechanisms [1]. The abundance of water, its non-toxicity and its capability to harden steel successfully were the main reasons of being the dominant quenching and cooling medium for thousands of years [2]. However, the high heat transfer rates raise the need for extra treatment in order to yield the preferred properties. A popular alternative for less severe heat transfer rates and reduced costs are mineral oils. However, oils tend to be a fire hazard, emit smoke, are difficult to safely dispose of and have a limited range in heat transfer rates [3].

Aqueous Polymer Solutions (APS) can successfully replace mineral oils to achieve the desired component metallurgical properties, while they are non-flammable, nontoxic, harmless to the operating personnel, easily removed from parts after quenching, and biodegradable. Nanofluids [4] are also affecting the wetting kinetics as well as heat transfer properties of the conventional fluids. Quenchants based on nanofluids can have increased thermal conductivity, increased stability, low erosion, low pumping power, etc.

The long term aim of this study is to characterise aqueous solutions containing polymers and/or nanoparticles with Molecular Dynamics (MD) in a range of concentrations and temperatures, from room up to 1100K. MD is a well-established simulation approach that is based on modeling the trajectory of molecules through interatomic potentials and Newton's law of motion. Unlike conventional Computational Fluid Dynamics, fluid and solid properties are not input parameters but measurable quantities. In this presentation we will introduce MD and show results for pure water assessing the accuracy of various water models proposed in the literature. An attempt will be also made to include preliminary results of aqueous solutions containing small polymer chains or nanoparticles.

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Investigation of the tunable character of the star-shaped polymer melts through chemistry-specific model

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In the recent years, the search for more sustainable and versatile materials with a wide range of rheological behavior resulted in an increase interest in all-polymer nanocomposites. The uniqueness of all-polymer nanofillers lies in their soft and tunable character, ranging from fully penetrable chain-like structures to particles which resemble conventional solid additives [1]. More specifically, star-shaped polymers, which are used as model systems for more complex architectures, represent an important member of this family of polymer objects, due to their well-controlled architecture, which facilitates the tuning of the dynamical behavior through the number of arms (functionality). A recent experimental evidence suggests that the internal packing may be another tuning factor [2].

In this work, we take advantage of the chemical specificity of atomistic molecular dynamics (MD) simulations and we study in detail structural and dynamical properties of non-entangled poly(ethylene oxide) (PEO) and polystyrene (PS) stars in melts. These two dissimilar polymers differ in flexibility and glass transition temperature. By varying the number of arms (functionality), we aim to alter the mutual penetration of the molecules and adjust the local packing. In addition to our previous structural analysis [3], we use two approaches to probe the dynamics with respect to the functionality. Firstly we investigate the dynamical behavior through the displacements of the center-of-mass of the molecules as well as segmental analysis along the arms [4]. The second approach involves the implementation of a challenging grid-based algorithm for the estimation of the free volume in the system, which is related to the permeability and T_g of the system. We focus our study on the distribution of the free areas around the center of the star and in this way extend the knowledge about the packing of the arms around the attachment point.

Our chemistry-specific results complement the results from experimental techniques or more generic theoretical models and can thus contribute to a better understanding of structure-dynamics relation in materials with branch-like architectures, such as those used in all-polymer nanocomposites or nanostructured electrolytes [5].

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A two-species model for the rheology of associative polymer networks from nonequilibrium thermodynamics

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We employ the generalized bracket formalism of nonequilibrium thermodynamics [1] to derive a constitutive model for reversibly-crosslinked networks of associative polymers, fluids that find extensive usages as rheology modifiers in a variety of commercial products today (health and personal care, enhanced oil recovery, paints and paper coatings, and many others) [2]. For these fluids, several important rheological models having been proposed over the years, mostly on the basis of separate contributions from bridges and (temporary) dangling chains [3-4].

A novel feature of the work presented here is that the expressions for the attachment and detachment rates as functions of applied flow and chain conformation arise naturally from the formalism. This is achieved by assuming a kinetic model [5, 6] for the formation / dissociation of chains from the network through, and is a big advantage compared to other efforts wherein these expressions are typically specified externally.

The final set of evolution equations obtained from our approach [7] are very similar to those of earlier models based on network kinetic theory, which is very nice given the totally different approaches followed (thermodynamics compared to polymer kinetic theory). A detailed analysis demonstrates the capability of the new model to describe various sets of rheological data for solutions of associative polymers [7].

A drawback of our new model is that it cannot predict the weak shear thickening observed experimentally prior to shear thinning in steady shear [8], despite the self-consistent incorporation of non-Gaussian effects in the attachment / detachment rates. According to Tripathi et al. [4], shear-thickening arises by allowing the detachment rate to be a function of the conformation of both bridges and dangling chains, leading to a shear-induced enhancement of bridges, but this cannot be accommodated in the current version of our model. We are currently working on this [9].

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POSTERS

High-frequency Optimally Windowed Chirp rheometry in fast evolving thermosets.

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We utilize frequency- and amplitude-modulated strain waveform in conjunction with a home-made sliding plate piezo-operated rheometer 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 render 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 sub-second scale. Therefore the duration of the scan is short compared to the evolution of moduli (mutation time) keeping the mutation number (N_{mu}) sufficiently low, even in fast evolving systems.

We provide proof of concept, by capturing the solidification of fast evolving soft matter composites such as a vinyl ester resin-fumed silica nanocomposite during curing process. The sol-gel transition is captured as the linear viscoelastic (LVE) spectrum is accessed almost every second portraying the rapid evolution of a frequency dependent moduli with adequate time resolution. Comparison of the Chirp application in commercial rotational and piezo based rheometer provides further information on the applicability of the technique.

High-pressure microrheology of supramolecular assemblies

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We present a methodology to investigate the linear viscoelastic properties of complex fluids at elevated pressures (up to 120 MPa) by means of passive microrheology. Dynamic light scattering is performed on a test sample within a stainless steel chamber, where the pressure is regulated by an inert gas. An application is to a hydrogen bonding motif 2,4-bis(2-ethylhexylureido)toluene (EHUT) in apolar solvents, forming different supramolecular structures (tubes and filaments), is presented. Increasing pressure slows-down the terminal relaxation time and weakly increases the entanglement plateau modulus and the persistence length. Increasing pressure in the tube regime may yield a transition from viscous (unentangled) to viscoelastic (partially-entangled to well-entangled state) solution. For well entangled, long tubes, the extent of the plateau regime increases with pressure. These findings can be summarized in the form of a temperature-pressure state diagram and provide insights for understanding and exploiting the role of pressure on the structure and dynamics of supramolecular polymers.

Hematocrit level-based assessment of turbulent-related wall shear stress of pulsatile blood flow in a pathological coarctation of the human aorta

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Assessing wall shear stresses (WSS) and the turbulent kinetic energy (TKE) map in a turbulent-like disturbed blood flow has become essential for evaluating the susceptibility and progression of vascular disease. These flow characteristics are frequently detected in regions of unfavorable anatomical obstructions such as pathological stenosis. Attention has been focused on magnetic resonance (MR), so far with limited success, promoting the need of WSS-based descriptors to characterize the spatiotemporal nature of the WSS disturbance with a differentiation between physiological laminar oscillations and turbulence-related oscillations, providing both a magnitude and an anisotropy measure of the disturbances; site-specific estimations of WSS disturbances in pulsatile transitional turbulent type of flows are more challenging due to continuous and unpredictable changes in WSS behavior.

In this work, an idealized geometry of pathological aorta's coarctation has been implemented, and Large Eddy Simulations (LES) along with the WALE sub-grid model is used to resolve the most energy-containing turbulent scale of the pulsatile flow, considering that previous works have highlighted the inability of RANS model for this kind of flows [1].

Under physiological conditions, blood is typically viscoplastic, i.e., it exhibits a yield stress that acts as a minimum threshold for flow, thus, rheological models such as Casson's one [2], parameterized on the red blood cell volume fraction (hematocrit) and fibrinogen concentration, is able to evaluate the deep rheological features of this kind of non-Newtonian fluid. The model under consideration covers a wide range of hematocrit and fibrinogen concentrations, thus can be adapted for patient-specific needs.

Furthermore, the results are used to investigate the difference between the aforesaid rheological model against other models. This enables the assessment of the role of the non-Newtonian behavior on the transition from physiological laminar to turbulent flow.

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Squeeze flow of thixotropic semisolid slurries

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The motivation for this work is the development of a numerical simulation model to predict the flow behaviour of semisolid metal slurries in thixofforming, a novel technology applied to produce complex near-net-shaped components with advanced mechanical properties. Semisolid materials behave as solids when

the applied stress lies below the yield stress and when the latter is exceeded, the material behaves either as a shear-thickening or as shear-thinning fluid with a non-linear stress-strain relationship [1-3]. In contrast to other thixotropic materials, semisolid slurries show partially irreversible rheological characteristics due to the breakage of the welded bonds between the particles [3, 4].

In the present work we model numerically the squeeze flow experiment of a semisolid material described by Herschel-Bulkley constitutive equation, using finite elements in Lagrangian coordinates. The compression is performed under constant load, applied on the top plate, while the bottom plate remains fixed. The yield stress is assumed to vary linearly with the structural parameter, which follows a first-order rate equation accounting for the material structure break-down and build-up. The development of the yielded/unyielded regions in relation to material structural changes is analyzed [3, 5].

The numerical model has been fitted against available experimental data on a semisolid aluminum alloy A356, where the sample is compressed from its topside under constant load at a temperature of 582°C while the bottom side remains fixed. The geometrical characteristics of the specimen used were 30 mm high (H_0 in m) and 30 mm in diameter and therefore a constant volume V was implied [6, 7]. Based on the load used in the experiments, we reproduce the compression flow numerically and the evolution of the sample height is studied for all the ranges of the Bingham and Reynolds numbers, the power-law exponent as well as the structure- kinetics parameters. Systematic comparisons have been carried out with the available experimental data. An agreement could be achieved provided that the load at the very initial instances is significantly higher than the load used by the experiment and that the power-law parameter varies with the structural parameter, which is consistent with the internal microstructure variations known to be exhibited by semisolid slurries.

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Steady sphere translation in an Oldroyd-B fluid with non-linear slip on the surface of the sphere

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We study analytically the effect of non-linear (quadratic) Navier type slip on the surface of a spherical particle which translates with constant velocity U in a viscoelastic polymeric ambient fluid. We assume steady state, isothermal and creeping flow conditions. The fluid is modelled with the Upper Convected Maxwell and Oldroyd-B constitutive equations. The solution for all the dependent flow variables is expanded as asymptotic power series with the small parameter being the Weissenberg number, $Wi = \lambda U/R$,

where λ is the single relaxation time of the fluid and R the radius of the sphere. The resulting sequence of equations is solved analytically up to fourth order in Wi . The effects of viscoelasticity (i.e., of the Wi number), the polymer viscosity ratio and the slip coefficient are presented and discussed. Comparison with the corresponding results for linear Navier slip on the surface of the sphere is performed and discussed too.

Torsional parallel plate flow of Herschel-Bulkley fluids with wall slip

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We consider the torsional parallel plate flow of Herschel-Bulkley fluids with wall slip. The latter is assumed to occur above a critical wall shear stress, the slip yield stress τ_c , taken to be lower than the yield stress, τ_0 [1]. When the rim shear stress τ_R is below the slip yield stress the exerted torque is not sufficient to rotate the disk and the material remains unyielded. When $\tau_c < \tau_R \leq \tau_0$ the material is still unyielded but exhibits slip and rotates as a solid at half the angular velocity of the rotating disk. Finally, when $\tau_R > \tau_0$, the material exhibits slip everywhere but yields only in the annulus $r_0 \leq r \leq R$, where r_0 is the critical radius at which the shear stress is equal to the yield stress. In the general case, the slip velocity, which varies with the radial distance, can be calculated numerically and then all quantities of interest, such as the true shear rate, and the two branches of the apparent flow curve can be computed by means of closed form expressions. Analytical solutions have also been obtained for certain values of the power-law exponent.

In order to illustrate the effect of wall slip on the apparent flow curve, we obtain results for different gap sizes between the disks choosing the values of the rheological and slip parameters to be similar to reported values for certain colloidal suspensions [2]. The computed apparent flow curves do follow the patterns observed in the experiments.

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Numerical study of the dynamic response of a liquid metal in a pore in the presence of a magnetic field and a heat load

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The unsteady flow arrangement of a liquid metal inside a single pore in the presence of a magnetic field is investigated numerically in order to determine its dynamic behavior when external heat and electric loads are applied on its interface. In the case of an azimuthal magnetic field and in the absence of a thermal load, a critical magnetic number is found ($Bondm = 4.5$) below which the flow reaches a steady state with mild rotational patterns. Above this threshold, the interface exhibits saturated oscillations. For $Bondm \geq 5.8$, a Rayleigh-Taylor instability develops that leads to drop formation¹. In the presence of a thermal load, the interface is stabilized since the onset of evaporation tends to suppress drop ejection. It is also found that

due to its higher surface tension Tin can withstand higher electric currents than Li in the absence of a thermal load or for thermal loads that do not cause boiling. In the case of an axial magnetic field and in the absence of a thermal load, there is a critical magnetic number $Bondm \approx 3600$ above which the flow exhibits a poloidal component at steady state besides the azimuthal swirling motion. The onset of interfacial instability is observed near the pore walls where intense swirling and poloidal motion are captured. In the presence of a heat load the instability is attenuated due to evaporation. The effect of spreading on the pore walls is also examined in order to assess its effect on the stability of the liquid metal layer. For complete wetting the Cox-Voinov theoretical prediction for the dynamic contact angle as function of spreading speed is recovered. The impact of liquid metal spreading along the pore walls against the drop injection effect that arises as a result of Lorentz forces, is currently investigated. The impact of plasma induced wetting on the stabilization of plasma reactors against drop ejection by using a capillary porous system as plasma facing component, is discussed.

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Rheology of reversible networks from star block copolymers

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In recent years, the exploitation of directional interactions has emerged as promising methodology to form reversible self-assembled multi-scale structures, with great significance in technological, energetic and biomedical applications. The state-of-the-art to date is the use of DNA constructs to introduce patchy interactions in materials. However, the DNA technology is often complex, and it is desired to combine material responsiveness with simplicity. We present here an alternative strategy to tailor the properties of physical networks through a synergetic use of macromolecular architecture and interactions. Stars with block copolymer arms having alternating block sequences in the same solvent represent the paradigm: telechelic star polymers (TSPs) containing attractive outer blocks self-assemble into soft patchy nanoparticles, whereas the inverted architecture with inner attractive blocks yields micelles. We focus on the concentrated regime where TSPs and micelles form bridged and interpenetrated hexagonally packed nanocylinders, respectively, and examine their structural and rheological properties. We construct phase diagrams and identify different regimes including amorphous liquid, ordered solid and re-entrant liquid, the latter being observed upon both heating and cooling, because of solvent-block and block-block interactions. Of particular interest is the region in the ordered phase characterized by the formation of nanocylinders. The interconnected nanocylinders networks exhibit enhanced storage modulus and extended structural coherence, which at the same time their maximum deformability at break (yield strain) is similar to that of interpenetrated structures, and similar to typical values of a wide range of colloidal depletion gels. On the other hand, they exhibit a much larger yield stress compared to micelles or typical colloidal gels. These results suggest that TSPs are a versatile building block for promising functional materials with tunable rheological properties.

Dynamic behavior of acoustically driven uncoated microbubbles near a wall: the microstreaming effects

The dynamic response of microbubbles without a protective coating is investigated subject to acoustic disturbances near a wall, in order to identify microstreaming effects around the bubble. These effects have been previously studied not only theoretically^{1,2} but also through experiments³. However, it has not been satisfactorily captured via numerical simulations. A parametric study is conducted numerically for a wide range of sound disturbances and liquid viscosities following a previous experimental study³. The flow domain is discretized spatially using the Galerkin Finite Element Methodology and the continuity and Navier-Stokes equations are employed for the description of the liquid. The interface with the surrounding liquid is characterized by surface tension. The simulations show that higher sound amplitudes resulted in an early collapse of the bubble, which failed to approach the wall and get trapped. For lower disturbances the bubble managed to reach the wall, get trapped as shown in Fig 1a,b, and produce microstreaming effects similar to those reported in the literature^{1,3}, Fig 1c. The amplitude of the radial pulsation is monitored (Fig. 1a), as a measure of the bubble-streaming Reynolds number. Simulations for higher values of viscosity allowed the bubble to get trapped for a wider range of amplitudes due to stabilization of the interface by viscous dissipation. Applications in ultrasonic cleaning are discussed.

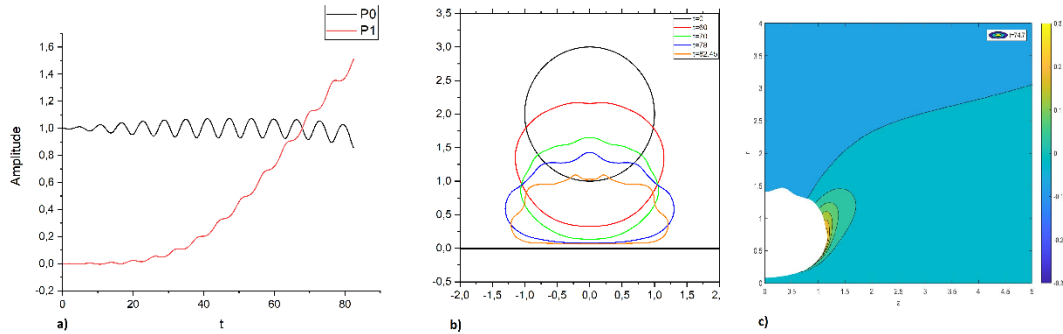


Figure 1: (a, b) Evolution of the bubble radial and translational motion and interfacial shape and (c) snapshot of the streamline pattern of a trapped microbubble; $\varepsilon=0.02$, $f=10\text{kHz}$, $R_0=300\ \mu\text{m}$, $\nu=10^{-6}\text{m}^2/\text{s}$, $\sigma=0.072\ \text{N/m}$

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Weakly nonlinear analysis of the effect of shell stiffness on the fundamental resonance of coated microbubbles

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The weakly nonlinear radial oscillations of a gas bubble that is encapsulated in an elastic shell are investigated by means of asymptotic analysis. The microbubble is immersed in an infinite, Newtonian fluid subject to a sinusoidal acoustic excitation in the far field. Viscous forces and compressibility effects, in the limit of small Mach number, are accounted for in the surrounding liquid. In this context, the Keller-Miksis model applies for the description of the nonlinear oscillatory motion of the bubble interface. Three different constitutive laws have been employed to describe the viscoelastic properties of the shell, which is taken to be free of prestress in the initial spherical equilibrium configuration. Namely, the Kelvin-Voight, Mooney-

Rivlin and Skalak models are used, pertaining to an almost linear for small displacements, strain-softening, and strain-hardening behavior of the material, respectively. Analytical solutions describing the steady-state oscillations have been obtained by regular asymptotic approximations, corresponding to the fundamental resonance of the bubble, that are valid to second order of approximation in terms of the sound amplitude. A parametric study is conducted, investigating the effect of the microbubble properties and ultrasound characteristics on the response of the interface to the imposed disturbance. The amplitude, as well as the resonance frequency of the fundamental harmonic, are monitored for each constitutive law governing the elastic behavior of the shell. The obtained results are displayed in the form of frequency response curves, Fig 1, of the steady-state pulsation for the different sets of parameters. When the membrane exhibits a strain-softening behavior the response curves shift to lower than the natural resonance frequencies as a result of nonlinearity, giving rise to the highest response amplitudes. When the material behavior is described as strain-hardening the opposite is true. The above pattern is corroborated by numerical studies¹ and complement previously reported asymptotic results obtained by different asymptotic methods^{2,3}, especially when weak damping mechanisms and lower forcing amplitudes are considered ensuring optimal implementation of the asymptotic scheme.

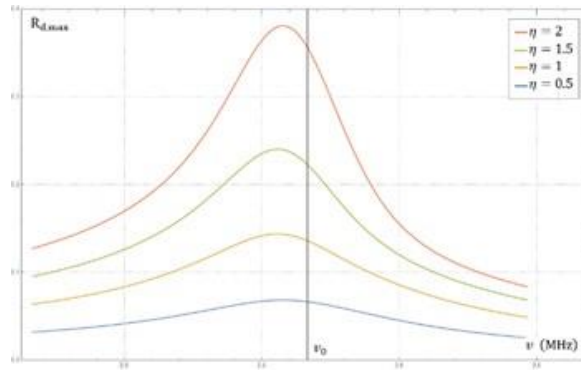


Figure 1. Frequency response curves for a strain softening (Mooney-Rivlin) type constitutive law for increasing amplitude of the external acoustic excitation.

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Crystallizing depletion colloidal gels by shear

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In this work we present the study of monodisperse attractive colloidal gels using both experiments (rheology and confocal microscopy) and molecular dynamics simulations. The system under study is a depletion gel of (nearly) monodisperse Poly-methyl methacrylate (PMMA) particles at large volume fraction (44%). The

attractive interactions are simulated using a Morse potential (harmonic oscillator with cutoff). We find that when such colloidal gels are sheared dynamically (i.e. applying oscillatory shear) they show a drop in their modulus(G) which depends on the applied strain amplitude (γ_0), frequency (ω) and shearing time, similarly to polydisperse colloidal gels, as previously reported [1]. More specifically, in both experiments and simulations the drop of the modulus depends non-monotonically on the strain amplitude, with the maximum decrease in the modulus appearing in the range of $\gamma_0=70$ to $\gamma_0=100\%$ depending on ω . At larger strain amplitudes, the modulus returns to a similar value as the quiescent gels suggesting that any structural transition responsible for the modulus drop occurring in the range of $\gamma_0\sim 100\%$ is destroyed for large strain amplitudes. In this range, MD simulations show that the gels undergo a crystallization transition, observed in similar systems before[2], which depends on the shearing time. At first, small crystallites are formed which later on grow into large crystalline domains, something that is also observed in the experiments using confocal microscopy coupled with rheology. The appearance of crystallization or not depends on both the frequency and the strain amplitude which can allow for tunability of the properties of the colloidal gel as well as the structure from a disordered to an ordered state but also suggests that it is connected with both some characteristic length scale and time scale of the system, and of course raises the question whether shear “pushes” the system toward equilibrium.

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