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Book of Abstracts



8th International Conference of the *Hellenic Society of Rheology*

12-14 July, 2017

Limassol, Cyprus

Message of the Organizing Committee

It is with great pleasure that we welcome all the delegates and accompanying persons to HSR 2017 (8th International Meeting of the Hellenic Society of Rheology, Limassol, July 12-14, 2017).

The 1st Meeting of the HSR was held in Cyprus, 21 years ago in Nicosia. Since then, the HSR meetings took place in Heraklion (1998 and 2014), Patras (2001), Athens (2004 and 2011), and Rhodes (2007). The main goal of these meetings is to promote scientific interactions at the highest level not only among the members of the Greek Chapter of the Society of Rheology but also among scientists from all over the World. Another objective of the meetings is to provide the forum where students could interact and share their work with the established members of the community.

The program includes three invited keynote talks by Professors Michel Cloitre (Paris Tech, France), Moshe Gottlieb (Ben Gurion University, Israel), and Fernando Pinho (Universidade do Porto, Portugal), 40 regular talks, and 13 poster presentations. With more than 50 registered participants from sixteen countries (Bulgaria, Canada, Cyprus, France, Germany, Greece, Iran, Ireland, Israel, Jordan, Luxemburg, Portugal, Russia, Switzerland, UK, and USA) the conference is truly an international event.

The workshop would not be possible without the financial support of the Department of Mathematics and Statistics and the Department of Mechanical and Manufacturing Engineering of the University of Cyprus, the Department of Mechanical Engineering of the Cyprus University of Technology, the Cyprus Tourism Organization, and the Cyprus Department of Antiquities. We are also grateful to the Paphos 2017 European Capital of Europe Organization, the Vouni Panayia Winery, and the Kamanterena Winery for their generous contributions.

We hope that *HSR 2017* will promote scientific exchange, collaboration and interactions between participants.

Georgios Georgiou and Andreas Alexandrou

PROGRAM

Tuesday, July 11, 2017	
19:30-21:30	Welcome Reception at Curium Palace Hotel (Venue)
Wednesday, July 12, 2017	
08:00-08:25	Registration
08:25-08:30	<i>Opening</i>
08:30-09:10	<i>Keynote lecture: M. Gottlieb, Interfacial rheology of block copolymers</i>
Chair: Dimitris Vlassopoulos	M.A.P. Mohammed, L. Wanigasooriya, S. Chakrabarti-Bell, M.N. Charalambides , <i>Extrusion of unleavened bread dough</i>
	T.D. Papathanasiou , <i>Permeability models for saturated fluid flow across random and aggregated fiber arrays</i>
	C. Saengow, A.J. Giacomin , <i>Oscillatory shear sweeps on complex fluids from the Oldroyd 8-constant framework</i>
	L. Gury , D. Vlassopoulos, M. Cloitre, M. Gauthier, <i>Searching for rheological signatures of jamming transition in soft hairy colloids</i>
	M. Das , G. Petekidis, <i>Flow induced vorticity aligned clusters of rod like particle suspension</i>
10:50-11:20	<i>Coffee break</i>
Chair: Yannis Dimakopoulos	N. Antonova , <i>Evaluation of blood clotting by rheological and electrorheological methods</i>
	I. Ivanov , N. Antonova, <i>The change of blood electrical conductivity - a marker for altered erythrocytes orientation under flow and electric field</i>
	I. Velcheva , N. Antonova, N. Chaushev, V. Paskova, S. Podtaev, K. Tsiberkin, <i>Skin microvascular tone regulation in diabetic patients: Relation to blood rheology</i>
	E. Kaliviotis , J.M. Sherwood, S. Balabani, <i>Red blood cell aggregate, shear and local viscosity distribution in bifurcating microscale blood flows</i>
	W. Al-Kouz , S. Kiwan, H. Saadeh, <i>Heat transfer analysis of rarefied flow in cavities with two fins attached to the hot-sided wall</i>
13:20	<i>N.A. Gatsonis, Non-isothermal smoothed dissipative particle dynamics for fluids in bounded mesoscopic domains</i>
16:00-16:30	<i>End of morning sessions</i>
Chair: Kostas Housiadis	<i>Poster Session - Coffee</i>
	I.Ch. Tsimouri , C.K. Georgantopoulos, P.S. Stephanou, V.G. Mavrantzas, <i>Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics</i>
	P. Panaseti , G.C. Georgiou, A.-L. Vayssade, M. Cloitre, <i>Confined viscoplastic flows with heterogeneous wall slip</i>
	D. Pasias , E. Kaliviotis, <i>Surface tension driven microfluidic blood flow: red blood cell aggregation and viscosity effects</i>
	D. Parisi , D. Vlassopoulos, B. Loppinet, Y. Ruan, C. Yang, <i>Shape effects on the rheological behavior of polymer-grafted nanoparticles in solution</i>
	K.D. Housiadis , G. Samanta, A.J. Young, A.N. Beris, <i>On the tails of probability density functions in Newtonian and viscoelastic turbulent channel flows</i>
	P.S. Stephanou , V.G. Mavrantzas, <i>Multi-scale modelling of high-MW polymer melt viscoelasticity starting from the atomistic level</i>
	P. Moschopoulos, Y. Dimakopoulos , J. Tsamopoulos, <i>Analytical expressions for the velocity field of polymeric fluids and polyelectrolyte in microchannels</i>
	S.M. Fayyad , <i>Using new magnetic rheological fluids in automobiles suspension systems - Comparison study</i>
	D.E. Apostolidis , C.S. Patrickios, E. Leontidis, T. Sakai, <i>Rheological investigations on dynamic covalent four-armed star poly(ethylene glycol) model hydrogels</i>
Chair: Kostas Housiadis	G.C. Florides , A.N. Alexandrou, M. Modigell, G.C. Georgiou, <i>Squeeze flow of thixotropic semisolid slurries</i>
	P.A. Panteli , C.S. Patrickios, <i>Synthesis and characterization of acrylamide-based dynamic covalent amphiphilic polymeric conetworks cross-linked via alkoxime bonds</i>
	E. Antonopoulou , C. Rohmann-Shaw, T. Sykes, O. Cayre, T. Hunter, P. Jimack, <i>Physical separation of colloidal systems</i>
	C. Machattos , M. Georgallas , C. Polydorou, E. Efthymiadou, T. Stylianopoulos, <i>Experimental analysis of nanoparticles binding through laminar flow between parallel plates</i>
	D.G. Tsakiris , P.V. Alatas, V.G. Mavrantzas , <i>Ring polymers: scaling laws and topological interactions based on detailed molecular dynamics simulations</i>
Chair: Kostas Housiadis	V. Harmandaris , A.N. Rissanou, P. Bačová, <i>Molecular simulations of graphene-based polymeric nanostructured materials</i>
	P.S. Stephanou , D.G. Tsakiris, E.N. Skountzos, V.G. Mavrantzas, <i>Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modelling coupled with NEMD simulations</i>
	E. Muravleva , <i>Application of machine learning techniques to viscoplastic flow modelling</i>
	Y. Dimakopoulos , G. Makrygiorgos, G. Georgiou, J. Tsamopoulos, <i>A fast and efficient algorithm for computing viscoplastic flows</i>
18:10	<i>End of afternoon sessions</i>
19:30-23:30	<i>Limassol city tour by bus and Banquet Dinner (Mezedopagida)</i>

Thursday, July 13, 2017	
08:30-09:10	<i>Keynote lecture: M. Cloitre, Bottlebrush polymers in colloidal suspensions and nanocomposites</i>
09:10-10:50	J. Vlachopoulos , <i>Modeling of sintering from rotational molding to additive manufacturing</i> H. Chakibi, I. Henaut , J.-F. Argillier, <i>Bubbles motion in polymer solutions: influence of rheology</i> A.N. Beris , P.M. Mwasame, N.J. Wagner, <i>Modeling the rheology of dilute emulsions</i> J. Laeuger , <i>New rheometric tools for complex materials</i> T. Athanasiou , D. Vlassopoulos, G. Petekidis, <i>Probing viscoelastic properties of complex fluids by piezo-rheometry in the intermediate frequency range</i>
Chair: Maria Charalambides	
10:50-11:20	<i>Coffee break</i>
11:20-13:40	X. Zhang, E. Lorenceau, T. Bourouina, P. Basset, F. Rouyer, J. Goyon, P. Coussot , <i>Wall slip: a lubricated frictional process?</i> E. Khoshbakhti, N. Golshan Ebrahimi , M. Khabazian Esfahani, <i>Prediction of long chain branching in uniaxial elongational flow</i> V.K. Konaganti, E. Mitsoulis , S.G. Hatzikiriakos, <i>The dependence of extrudate swell on rheological parameters</i> E. Chatzigiannakis , M. Ebrahimi, M.H. Wagner, S.G. Hatzikiriakos, <i>Wall slip and melt fracture of polyisobutylenes</i> S. Costanzo, D. Vlassopoulos , <i>Attempts to measure shear viscosity and normal stresses in polymer melts</i> A. Louhichi , V. Metri, J. Yan, K. Matyjaszewski, W. Briels, D. Vlassopoulos, <i>Dynamics of associating star polymers with self-healing performance, studied by rheology and Brownian dynamic simulation</i> G. Petekidis , <i>Flow of colloidal gels and attractive glasses. Comparing experiments with computer simulations</i>
Chair: Thanassis Papathanasiou	
13:40-14:15	<i>Poster session & HSR Executive Meeting</i>
14:15	<i>End of morning sessions</i>
15:30-22:00	<i>Excursion to Curium and Paphos</i>

Friday, July 14, 2017	
08:30-09:10	<i>Keynote lecture: F. Pinho, Turbulence models for non-Newtonian fluid flows</i>
09:10-10:50	A. Kalogirou , M.G. Blyth, D.T. Papageorgiou, <i>Surfactant destabilisation in thin-film shear flows</i> P.K. Ray , T.A. Zaki, D.T. Papageorgiou, <i>Linear stability of viscoelastic oscillatory shear flow</i> D.T. Papageorgiou, P.K. Ray , J. Hauge, <i>Weakly-nonlinear interfacial instabilities in two-layer viscoelastic Couette flow</i> A. Lytra , K. Efthimiou, M. Vlachomitrou, N. Pelekasis , <i>Static and dynamic response of coated microbubbles</i> K.D. Housiadas , <i>Improved convergence based on linear and non-linear transformations at low and high Weissenberg number</i>
Chair: Vagelis Harmandaris	
10:50-11:20	<i>Coffee break</i>
11:20-13:40	G. Makrygiorgos, D. Fraggedakis, Y. Dimakopoulos, J. Tsamopoulos , <i>Structural processes in elastoviscoplastic materials</i> L. Muravleva , <i>Squeeze axisymmetric flow of a viscoplastic Bingham medium</i> D.M. Salmanidou, A. Georgioupolou, S. Guillas, F. Dias , <i>Rheological considerations for modelling of submarine mass failure processes at the Rockall Bank</i> H. Huang , A. Zilian, <i>Numerical prediction of the rheological properties of fresh selfcompacting concrete</i> A. Syrakos , Y. Dimakopoulos, J. Tsamopoulos, <i>Flow in a fluid damper: investigation of the effects of shear thinning and viscoelasticity through numerical simulations</i> P. Panaseti, Y. Damianou , K.D. Housiadas, G.C. Georgiou, <i>Analysis of pressure-driven flow in long channels of a Herschel-Bulkley fluid with pressure-dependent rheological parameters</i> E. Klerides , N. Kanaris, F. Stylianou, S. Kassinos, A. Alexandrou, <i>The lock-on regime in the wake of a periodically perturbed flow of a viscoplastic fluid past a confined circular cylinder</i>
Chair: Evan Mitsoulis	
13:40	<i>End of HSR2017</i>

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J. Tsamopoulos, Greece
D. Vlassopoulos, Greece

INVITED TALKS

Interfacial rheology of block copolymers

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Amphiphilic block copolymers have been recognized as effective surface active molecules with multitude of industrial and medical applications. Yet, the relationship between the molecular architecture, size and chemistry and the interfacial properties is not clear. Fundamental understanding of these simpler molecules may provide the tools for understanding interfacial behavior of structurally more complex biopolymers. Adding functionalities to these molecules widens the range of possible applications and responsiveness of the molecules to environmental conditions.

In this study, we examined a series of diblock and triblock copolymers of different sizes and compositions at different interfaces. These highly amphiphilic copolymers show some remarkable features. The experiments carried out here focus on the effects of architecture (diblock vs. triblock), chain length, block size and block size ratio (A/B) on the dynamics and rheology of the interfaces. Special attention is devoted to the differences between the results obtained by different rheological experiments.

Despite the great progress made in the last decade in interfacial rheometry several issues are still unresolved. In contrast with bulk rheology, in many cases there is a large discrepancy between results obtained by different rheological experiments. Oscillating pendant drop is a popular experimental technique for the study of interfacial rheology due to its relatively simple implementation [1]. Recently, arguments have been raised regarding the analysis of the results obtained by this technique. Most importantly, the lack of correspondence between experimental values obtained by dilatational and by shear interfacial experiments. In addition, it has been argued that in complex interfaces such as in the presence of surfactants or macromolecules, the complex structure on the interface results in an anisotropic interfacial stress tensor which may include shear rather than purely dilatational components [2, 3]. In addition, concerns based on the aspherical shape of the droplet, the effect of curvature have been mentioned. To explore some of these issues we have carried out a series of experiments comparing interfacial properties obtained by different techniques.

Finally, in quite a few oscillatory experiments non-linear effects manifested as even higher harmonics have been observed. Several such examples will be presented.

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Bottlebrush polymers in colloidal suspensions and nanocomposites

Michel Cloitre

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Bottlebrush polymers are high molecular weight macromolecules consisting of a polymeric backbone densely tethered with long side chains. The conformation of bottlebrush polymers is controlled by the steric repulsion between the lateral chains. This remarkable architecture is wide-spread in biomacromolecules like proteoglycans, where it is at the origin of unique functional properties. Important examples include aggregating proteoglycans, which in articular cartilages behave like micro-sponges controlling shock absorption and joint lubrication, and proteoglycans of the pulmonary mucus, which contribute to the mucociliary clearance of lung airways.

Recently bottlebrush polymers have become accessible to modern synthetic techniques. In this lecture, we will focus on a class of polyelectrolyte copolymers obtained by a grafting-through method, which consists in the direct polymerization of well-controlled macromonomers. In solutions, these bottle brush polymers have a low viscosity up to high concentrations, are insensitive to pH or ionic strength variations, and exhibit a rich microscopic dynamics. They have interesting applications when they are mixed with colloids. When added to nanocomposites at low concentrations, they provide high resistance to mechanical compression, reduce the permeability of water, enhance water retention, and produce uniform defect-free patterns after drying. We will show how this synergy of properties, which is reminiscent of those of bottlebrush biopolymers, is directly connected to the specific architecture of the macromolecules and to their ability to develop specific interactions with colloids.

Turbulence models for non-Newtonian fluid flows

F.T. Pinho

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The use of additives that impart non-Newtonian characteristics to an otherwise Newtonian solvent has the potential to reduce friction in turbulent pipe flow by as much as about 80%. This has triggered a wealth of research over the last 70 years, but the development of turbulence models for engineering design, that are consistent with rheological constitutive equations, has really only started some 20 years ago. We review the current knowledge on the characteristics of some canonical turbulent flows, such as fully-developed pipe/channel flow, but also isotropic turbulence or planar jet flows, obtained through experiments and direct numerical simulations with polymer solutions, and then we proceed to give an overview of existing turbulence models for engineering purposes in the context of RANS (Reynolds average Navier-Stokes), but also in the context of LES (large eddy simulation) where the next generation of models are likely to appear.

Acknowledgments

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REGULAR TALKS

Extrusion of unleavened bread dough

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An experimental and numerical study on ram extrusion of bread dough was conducted in order to develop predictive models for the pressures involved, as well as the deformation of the extruded dough. Such studies are needed as high pressures can potentially lead to significant degassing, tearing and shearing of the dough and hence poor bread quality; the latter limits the use of extrusion processes which would otherwise be a cost – effective forming process. Rate dependent behaviour was observed from tests conducted at different extrusion speeds, and higher extrusion pressure was reported for dies with smaller exit radius or larger die angle. A simulation of extrusion was performed to predict the extrusion pressure as well as the extrudate swell, as a function of die geometry and extrusion rate. A nonlinear viscoelastic model combined with the Mullins model for filled rubbers is found to capture the continuum behaviour well. A Coulomb friction law combined with a maximum shear stress limit was used to describe the contact definition between the extrusion barrel and the dough. Higher die angles and higher extrusion speeds require higher shear stress limit values for the model and the experiments to agree. The onset of the static zones was predicted well but quantifying the geometry of the latter needs further studies.

Permeability models for saturated fluid flow across random and aggregated fiber arrays

T.D. Papathanasiou

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We investigate computationally the effect of randomness as well as the effect of fiber aggregation on the hydraulic permeability (K_{eff}) of unidirectional fiber arrays. For this we carry out extensive viscous flow computations in various structured and un-structured fiber arrays. Two types of fiber arrays are considered; in the first, the fibers are assumed to be clustered in square or hexagonal packing. Simulations show that the effective permeability of such arrangements can be expressed by an empirical formula in terms of the intra- and inter-tow porosities. In the second case, we consider random fiber arrays which are generated through a Monte-Carlo process, starting from uniform square arrays or from regular arrays of fiber clusters. Up to 900 individual fibers are included in each simulation. The results demonstrate that at high values of (ϕ), deviations from the uniform array result in a decrease of K_{eff} . At lower porosity levels, the permeability shows a maximum at some intermediate value of the mean Nearest Neighbor Distance (\bar{d}_{nn}). It is shown that fully clustered fiber arrays have higher K_{eff} than randomized ones; it is also shown that for these systems (K_{eff}) scales with the deviation of Ripley's second order intensity function for the given microstructure from that of the Poisson distribution. Finally, we propose a metric of the aggregation state of the fiber assembly which appears to correlate with the computed permeability.

Oscillatory shear sweeps on complex fluids from the Oldroyd 8-constant framework

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Large-amplitude oscillatory shear flow (LAOS) is a popular experiment for studying the nonlinear physics of complex fluids. Specifically, the strain rate sweep (also called the strain sweep) is used routinely to identify when a complex fluid begins to exhibit nonlinear behavior. In this paper, we give the exact expressions for the nonlinear complex viscosity and the corresponding nonlinear complex normal stress coefficients for the Oldroyd 8-constant framework evaluated for LAOS. We choose the Oldroyd 8-constant framework for its rich diversity of popular special cases (we list 18 of these). We evaluate the Fourier integrals of our previous exact solution to get exact expressions for the real and imaginary parts of the complex viscosity, and for the complex normal stress coefficients, as functions of both test frequency and shear rate amplitude. We explore the role of infinite shear rate viscosity on the strain sweep responses for the special case of the corotational Jeffreys fluid. In our Worked Example, we use this special illustrate the reality of our exact expression for the magnitude of the complex viscosity on the strain sweep response. We find that increasing η_∞ raises the real part of the complex viscosity, and decreases its imaginary part.

Searching for rheological signatures of jamming transition in soft hairy colloids

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Recently, dense microgel suspensions were shown to exhibit a glass-to-jamming transition characterized by larger yield stress and strain and stronger dependence of plateau modulus on concentration for the jammed state. As these microgels have almost no dangling ends, a natural question is the role of grafted arms of soft colloids (allowing for interpenetration) on this transition. In this work we address this challenge. In particular, we investigate the rheological behavior of highly concentrated solutions of 800-arm star polybutadiene (1,4-addition) in the nearly-athermal solvent squalene. We perform transient shear (step rate) experiments and investigate both the build-up of stress and the subsequent relaxation upon flow cessation, as function of both concentration (0 to 100% wt) and shear rate (5×10^{-4} to 10 s^{-1}). As model systems, star polymers exhibit a rather well-understood soft interaction potential that depends on the number of arms. Concentrations up to the melt were investigated, hence spanning the gap from solution to melt, while maintaining a moderate plateau modulus (in the order of 100 kPa). Plateau modulus, yield stress and other rheological properties are also investigated against concentration in search for a possible jamming transition inside the glassy regime ($C >> C^*$). The results provide a rather complete experimental test that can serve as basis for understanding the interplay of softness (reflected in interpenetration and shrinkage) and the potential jamming transition throughout a very wide range of concentrations.

Flow induced vorticity aligned clusters of rod like particle suspension

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Rod like colloidal particle suspensions exhibit a much richer phase diagram compared to their spherical counterparts. They form additional “Liquid Crystalline” (LC) phases with structural properties in between that of a liquid and a crystal. These phases have interesting rheological properties.

Here we study the rheological effects of flow induced clustering of dilute suspensions of silica rods ($L \approx 5 \mu\text{m}$, $d = 0.4 \mu\text{m}$) in CsCl solution (65 wt%). The rods possess attractive van der Waals interaction introduced by screening of their negative surface charge by counter-ions from CsCl solution and the suspension exhibits a weak gel like behaviour. Using different visualization techniques (light scattering, microscopy) along with rheological measurements, we observe shear induced cluster formation in the vorticity direction. Higher shear rates for extended durations however, result in the destruction of these clusters and leads to a phase separation which leads to a liquid like response. We show the effect of parameters such as particle concentration, shear rate, tool geometry and gap settings on the dimensions of the clusters. Interestingly the flow induced cluster formation can be avoided in samples with specific pre-shear history: once presheared at high rates the system does not form clusters at low shear rate. We also observe that for a system without preshear history, a shear thickening regime at very high shear rates exists. Furthermore, using confocal microscopy we attempt to explore the 3D positional and orientational ordering of individual rods under different flow regimes.

Evaluation of blood clotting by rheological and electrorheological methods

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A number of investigations revealed the role of the blood viscosity changes and the principles of the mechanical force applying and detecting the response of coagulating blood in terms of clot elasticity, rouleaux size and the rate of coagulation - a phenomenon, consisting of a number of sequential conversions of plasma constituents resulting formation of a blood clot.

The changes in the rheological behaviour of normal blood conserved by CPD-A₁ under conservation at a steady and oscillation flow conditions have been studied. The process of clotting was initiated *in vitro* and the kinetics of clot formation, viscous and viscoelastic properties of blood clot have been evaluated. The experiments were carried out by the rotational viscometer Low Shear 30 (LS30) Contraves as a base unit. Viscous and elastic component (storage modulus) of the complex viscosity were measured with Low Shear 30 sinus Contraves viscometer.

Clotting of stored blood was investigated by electrorheological method too. Blood viscosity and conductivity changes with the evolution of the coagulation process and under shear were also measured simultaneously. The coagulating sample was tested at a steady shear flow at two shear rates 0.0237 s^{-1} and 0.0596 s^{-1} . For the purpose which LS30 viscometer is connected with a specially developed conductivity measurement device. Both are joined with PC with special software for measurement of conductivity of biological liquids. This laboratory setting allows to be measured simultaneously with the rheological and electrical properties of the liquid, in particular the electrical conductivity.

It was found that the apparent viscosity of the stored blood has been elevated during conservation. This elevation was more pronounced at lower than 5.96 s^{-1} shear rates and after

the 22nd-25th day of conservation. Rheological coagulation test gives information about the kinetics of whole blood clot formation at defined flow conditions. The viscosity growth function (viscosity vs. time) at a constant shear rate have been determined and an exponential growth was established at shear rates from 0.0175 s⁻¹ to 1,25 s⁻¹ after recalcification solution addition.

The dependence between the elasticity modulus and the viscous component of the complex viscosity and the storage modulus on the frequency under the oscillation sinusoidal viscometric flow have been determined after 30 minute conservation at rest.

It is found that the clot formation is accelerated by the intensity of flow. The tendency of higher rate of coagulation at the same flow conditions during 35 days' conservation period is observed. Hemocoagulation kinetics research demonstrated a decrease of the blood clotting time during storage period.

References

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The change of blood electrical conductivity - a marker for altered erythrocytes orientation under flow and electric field

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Red blood cells (RBCs) under flow change their orientation and deformability in dependence of different factors as shear rate, hematocrit, erythrocyte rheological and morphological properties, plasma viscosity. Our previous studies show that blood electrical conductivity (BEC) under flow strongly depends on the same factors at Couette shear flow. The different levels of RBCs orientation lead to different electrical conductivity of the blood samples in different flow axes - it has electrical anisotropy. The aim of our study is to show the relationship between RBCs orientation at different flow regimes and blood electrical conductivity (BEC). The results show that BEC change strongly depends on the inner structure, which is formed by RBCs aggregates at low shear rates and by a smaller aggregates or single RBCs at high shear rates. BEC also depends on shear rate and on the duration of shearing at different flow regimes. Elevated BEC was obtained with increasing shear rate suggesting increased RBCs orientation along the streamlines. The results demonstrate that BEC change is strongly dependent on the inner structure alterations and on RBCs orientation and deformation respectively.

Skin microvascular tone regulation in diabetic patients: Relation to blood rheology

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The wavelet transformation analysis was used to study the localized variations of the low amplitude oscillations of skin temperature in accordance with myogenic (0.05 – 0.14 Hz), neurogenic (0.02 – 0.05 Hz), and endothelial (0.0095 – 0.02 Hz) control mechanisms and their association with skin blood flow changes during indirect cold test in 10 patients with diabetes mellitus type 2 and 10 healthy age and sex matched controls.

Skin temperature and blood flow of the volar side of the distal phalange of the 2nd finger were continuously measured under basal conditions (10 min), during contralateral hand immersion in cold water (3 min) and thereafter (10 min). The amplitudes of the skin temperature pulsations (ASTP) were monitored by means of thermistor sensor of the “Microtest” device (“FM-Diagnostics”, Russia). The whole blood viscosity (WBV) and the shear stresses were measured by Contraves LS30 viscometer, (Switzerland) at a steady flow in 10 healthy subjects and in 30 patients with type 2 diabetes mellitus. The basic hemorheological constituents as hematocrit (HT), fibrinogen (FIB) and plasma viscosity (PV) were also investigated.

Power law and Herschel-Bulkley (HB) equations were applied to describe the blood rheological properties and flow curves. Both models include consistency (k) and flow index (m), and the HB also gives the yield stress (τ_0). The Spearman rank correlations between these parameters and the ASTP in the frequency ranges, corresponding to the myogenic, neurogenic and endothelial mechanisms of the microcirculation tone regulation were calculated.

During the cold stimulus significant reduction of the temperature fluctuations in the neurogenic and endothelial frequency bands in the diabetic patients was established. Significant increase of Ht and WBV at shear rates of 0.0237 s^{-1} to 128.5 s^{-1} in the patients in comparison to controls was found. The ASTP values decreased when the blood viscosity increased. The correlation analysis revealed good ASTP– m ($r>0.5$) and ASTP– k ($r<-0.5$) relationships in the endothelial range, while the ASTP– τ_0 correlation was weaker ($r\approx-0.4$). These correlations became lower for the ASTP during the cold stress.

The results prompt manifestation of endothelial dysfunction associated with increase of the blood viscosity values in the patients with type 2 diabetes.

Red blood cell aggregate, shear and local viscosity distribution in bifurcating microscale blood flows

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The red blood cell aggregation phenomenon is majorly responsible for the non-Newtonian nature of blood and is present in a number of pathological conditions, influencing the flow characteristics in the microvasculature. It has been recently shown that red blood cell aggregation affects, among other characteristics, the aggregate distribution in bifurcating geometries in a counterintuitive manner. That is, the smaller aggregates appear in regions of lower shear, contrary to the general understanding that aggregation increases at these shear

conditions. This behaviour was attributed to (a) the existence of regions depleted by aggregates of certain sizes in the feeding branch, and (b) to the change in the exact flow split location in the same branch, which is altered according to the flow conditions in the outlet branches. In this work the local viscosity distribution in a T-type bifurcating channel is analysed based on an aggregation- and haematocrit- (among other parameters) dependent constitutive equation for blood, developed earlier by one of the authors (*Biorheology* 46 (2009) pp.487-508 and 48 (2011), pp. 127-147). The shear fields in the channel are estimated based on the aggregate size – shear rate relationship, as derived from relevant experimental work. The trends show that in the branches of lower flow rate the local viscosity is also, low helping to explain why the effects of physiological red blood cell aggregation are not destructive in terms of *in vivo* vascular resistance.

Heat transfer analysis of rarefied flow in cavities with two fins attached to the hot-sided wall

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The fluid flow and heat transfer in a buoyancy driven rarefied flow in a cavity heated from the side while attached to two fins is numerically investigated. Cavities are of interest in evacuated solar collectors to reduce heat loss from the system. This research provides a useful information to estimate heat transfer in low pressure cavities. The governing equations along with the slip flow and temperature jump boundary conditions are solved using the finite-volume technique. Effects of Knudsen number, Rayleigh number, and the length of the fin on the heat transfer characteristics is investigated and discussed.

Non-isothermal smoothed dissipative particle dynamics for fluids in bounded mesoscopic domains

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The Smoothed Dissipative Particle Dynamics (SDPD) method was introduced by Espanol and Revenga [1] as a top-bottom approach and thermodynamically consistent alternative to DPD. We review our work on a non-isothermal SDPD development and implementation with dynamic virtual particle allocation (SDPD-DV) for liquids and gases in arbitrary wall-bounded domains. The particle entropy for monatomic and diatomic gases, is evaluated through a Sackur-Tetrode type of equation, which in turn provides the internal energy. For liquids, the entropy and the internal energy are given as a second-order expansion using the coefficient of volumetric thermal expansion and of adiabatic compressibility. The particle pressure and temperature are calculated by thermodynamic relations. The integration of position-momentum SDPD-DV equations was accomplished with a velocity-Verlet (VV) algorithm. Bounce-forward is added to the velocity-Verlet integrator when needed to fully prevent particle penetration. The integration of the entropy SDPD-DV equation is accomplished with an implementation of the Runge-Kutta algortihm. The dynamic virtual particles allow the implementation of Dirichlet and Neumann thermal boundary conditions. The sampling methods used in SDPD-DV for particle, fluid (macroscopic) properties, hydrodynamic fluctuations, the self-diffusion and viscosity coefficients are presented. The theoretical hydrodynamic fluctuations are summarized. The paper presents an extensive set of SDPD-DV simulations of liquid water, argon gas and diatomic nitrogen gas equilibrium

systems used for validation and verification of our implementation. The SDPD-DV derived density, temperature, pressure, self-diffusion coefficient, shear viscosity, and hydrodynamic fluctuations are compared with analytical and experimental values.

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Ring polymers: scaling laws and topological interactions based on detailed molecular dynamics simulations

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Ring polymers, which completely lack chain ends, exhibit conformational and viscoelastic properties that differ considerably from those of the corresponding linear or branched polymers. Over the past decade, considerable progress has been made in elucidating several aspects of these properties with experimental techniques such as small angle neutron scattering (SANS), neutron spin echo (NSE), and pulse-field gradient NMR and rheology.¹⁻² Molecular simulations have also been very helpful in this direction.³

In this work,⁴⁻⁵ we will present results from detailed molecular dynamics (MD) and nonequilibrium molecular dynamics (NEMD) simulations of model ring poly(ethylene oxide) (PEO) melts with molecular weights in the crossover region around the characteristic entanglement molecular weight (MW) of linear PEO. Properties to be discussed include: a) the radius-of-gyration, b) the diffusivity, c) the dynamic structure factor, and d) the viscosity (as well as the rest of viscometric functions in simple shear). We will carry out a direct comparison with the corresponding properties of linear counterparts and with available experimental data, and we will extract their scaling with MW. How topological constraints (e.g., due to ring-ring threading)⁴ affect these properties both at equilibrium and out of equilibrium (flow) will be also discussed.

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Molecular simulations of graphene-based polymeric nanostructured materials

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Graphene-based polymeric nanostructured systems and van der Waals heterostructures comprise a material class of growing technological and scientific importance, which have attracted great attention the last years.^[1-5] The aim of our work is to examine spatial and dynamical heterogeneities of graphene based polymer nanocomposite systems and to provide information about their properties for various (edge group functionalized) graphene sheets. Pristine graphene and two types of functionalized graphene have been simulated in two different polymer matrices, (polyethylene, PE) and (polyethylene oxide, PEO). Systems are studied through detailed atomistic Molecular Dynamics (MD) simulations.^[2,3]

Furthermore, we analyze the conformational transitions, such as wrinkling and rippling, of graphene sheets with nm dimensions (nanographene) dispersed in a polymer matrix at equilibrium as well as under external stimuli (i.e. strain). Results about the conformational-morphological transitions of the graphene layers (rippling), as well as about its anisotropic Brownian Motion are presented.^[4]

Finally, we provide a detailed study of the structure and dynamics of a single-chain polymer crystal adsorbed on graphene under equilibrium and non-equilibrium conditions.^[5] In equilibrium, the adsorbed polymer is orientationally linked to the graphene as two-dimensional folded-chain crystallite or at elevated temperatures as a floating solid. The associated superstructure can be reversibly melted on a picosecond time scale upon quasi-instantaneous substrate heating, involving ultrafast heterogeneous melting via a transient floating phase.

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Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modelling coupled with NEMD simulations

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Polymer matrix nanocomposites (PNCs) are formed by adding nanoparticles (NPs) to a polymer matrix. In the present work, we propose a multiscale approach to study the rheology of PNCs with spherical inclusions by coupling a rheological constitutive model developed on principles of nonequilibrium thermodynamics [1] with non-equilibrium molecular dynamic simulations (NEMD). The mesoscopic rheological model for PNCs has been developed initially for unentangled polymer melt nanocomposites [1,2] and has provided a very satisfactory description of available experimental data regarding the phase behaviour [3], conformational properties and rheological [4] properties of these materials. In the absence of chain elasticity, the new model reduces to the Jeffery constitutive equation for the rheology of a Newtonian suspension of spheroidal NPs. The model addresses NPs of spherical shape by constraining the orientation tensor to be always equal to its equilibrium value, and provides predictions for the phase behaviour and rheological properties in shear that are consistent with experimental data.

In a second step, atomistic NEMD simulations are carried out with model PNCs systems similar to those used in experimental studies in order to get estimates of the values of the parameters appearing in the mesoscopic model. Key among these parameters is the longest polymer chain relaxation time and its dependence on the volume fraction of NPs. Additional parameters refer to the degree of interaction between polymer chains and NPs or between NPs and NPs. Our combined theoretical-simulation work provides a unified approach to the phase behaviour, chain conformation, swelling and rheological properties of PNCs melt, as a function of NP volume fraction, NP size, and imposed deformation rate.

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Application of machine learning techniques to viscoplastic flow modelling

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Yield stress fluid flows play an important role in the oil and gas industry (see recent review by Frigaard et. al [1]). There are many numerical methods for modelling such flows, and they often are computationally expensive. In this work, we propose to reduce computational complexity of parametric studies of Bingham fluid flows by utilizing machine learning techniques. The idea is as follows: instead of solving the PDE for each parameter value, we first do several simulations for a few scenarios (build a training dataset), construct a surrogate model to predict the solution for any parameter value. In this case, we have much faster model.

We apply this approach to a well-known Mosolov problem with Bingham number as a parameter.

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A fast and efficient algorithm for computing viscoplastic flows

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Efficient computation of viscoplastic fluids flows has always been a daunting task in the literature. Viscoplastic models are intrinsically discontinuous at the liquid-solid interface and this leads to numerical difficulties. For this reason, several numerical approaches have been proposed with the most popular being the Papanastasiou regularization [3] and the Augmented Lagrangian method [5]. Recently, studies have been intensified in order to develop accelerated algorithms [4], since the aforementioned methods possess a high computational cost and their results may lack the physical validity that is required. In the present work, a fast and efficient algorithm is proposed for accurately tracking the yielding surface and thus predicting the flow field of Bingham type fluids flows. The numerical procedure which is implemented is based on a monolithic Newton's solver. In order to test our algorithm, several benchmark flow problems are being studied. A pioneering study in the field is the paper of Beris et al., 1985 where the problem of a falling sphere in a Bingham medium is examined and serves as validation test. Similarly, we solve the problem of the steady rise of a bubble in a Bingham medium and validate our algorithm based on the findings of Dimakopoulos et al., 2011. Another important flow which is studied is the rectangular channel flow where a plug region is expected in the center and the corners of the domain. Finally, the transient filament stretch of a Bingham material is examined. The algorithm is able to capture correctly the yield surface that is formed, while maintaining a low computational cost since the convergence of the method requires only a few iterations.

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Modeling of Sintering from Rotational Molding to Additive Manufacturing

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Rotational Molding (RM) is a process for the production of parts by heating of polymeric powders in a bi-axially rotating mold, melting, particle coalescence, densification, cooling and solidification. The crucial step is the coalescence process (usually referred to as sintering)

driven by surface tension and opposed by viscosity. Most of the evidence suggests that elasticity slows down coalescence, which is quantified by the rate of neck growth. Polymers having zero shear viscosity higher than about 5,000 Pa.s are not rotomoldable. Modeling is based on Frenkel's model, applicable for the early stages, which has been extended to completion. Selective Laser Sintering (SLS) is an additive manufacturing technology for parts production in a layer-by-layer manner. In SLS a laser source is used to locally heat fine powder particles, which are subsequently subjected to coalescence, densification and solidification. The extended Frenkel model is also applicable for the description of neck growth in SLS. In this process, in addition to the relatively low viscosity, a temperature operating window (interval between the temperatures for onset of melting and densification) is required. Fused Deposition Modeling (FDM) is another additive manufacturing technology in which a molten filament is extruded from a miniature heated nozzle and deposited on a platform. Again, the process of neck growth, between adjacent filaments, can be described by the balance of surface tension and viscosity (extended Frenkel model). Modeling of sintering in FDM is further complicated due to the extrudate swell phenomenon. Better rheological characterization of polymers and improvements in modeling of neck growth and densification phenomena can lead to broader choices of suitable materials, reduction of cycle times and improvement of end-use properties.

Bubbles motion in polymer solutions: influence of rheology

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Oil extraction generates large amounts of water discharges. Several processes (centrifugation, filtration, flotation etc.) are deployed to remove residual oil droplets from these effluents and limit their environmental impact. Anyhow, these technologies are significantly challenged when polymer is injected in the reservoir rock to improve oil recovery. As a result the aqueous effluents to treat are no longer low viscous Newtonian but elastic, highly viscous and even shear thinning fluids. The impact of these rheological changes has been investigated for flotation which principle is to accelerate the creaming of oil droplets by combining them with rising gas bubbles. We studied the bubbles flow patterns in polymer solutions using a lab scale flotation column. They evolve from small, well dispersed and independent bubbles (Figure 1a), to preferential ways and bubble clusters (Figure 1b) as polymer concentration increases. This phenomenon is often attributed to the solution elasticity [1,2] while a strong shear-thinning behavior exists. So, we propose here to discuss the relative contributions of elasticity and shear-thinning to the bubble flow modification. In addition, we studied the respective motion of bubbles formed with a capillary to follow the rising of successive bubbles and the appearance of clusters [3]. The results have been analyzed with respect to the rheological characterization of the polymer solutions performed in shear and in extensional flows.

The attachment between a bubble and an oil droplet separated by an aqueous phase constitutes a complex interfacial phenomenon that also governs the efficiency of flotation. We have shown that this interfacial process is affected by the presence of polymer.

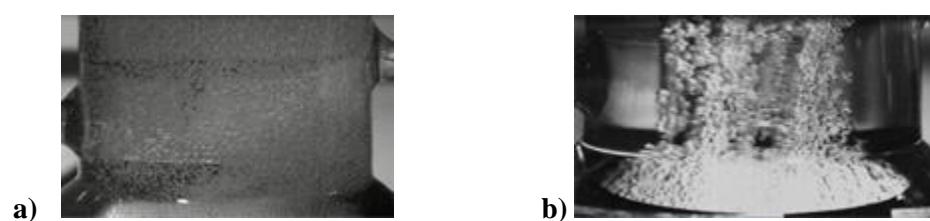


Figure 1: Bubble flow a) in dilute regime: bubbles homogeneously dispersed; and b) at high concentrations of polymer: jet of bubbles

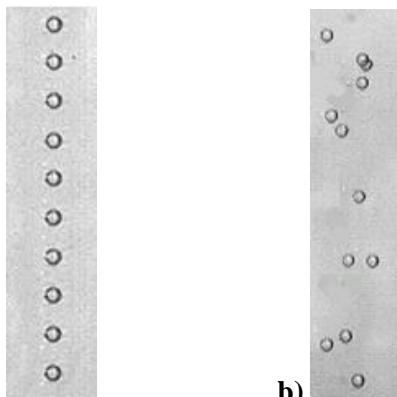


Figure 2: Bubbles rising in a) a Newtonian fluid and in b) a shear thinning fluid

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Modeling the rheology of dilute emulsions

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A new macroscopic model describing the rheology and microstructure of dilute emulsions with droplet morphology is developed based on an internal contravariant conformation tensor variable which is physically identified with the deformed ellipsoidal geometry of the dispersed phase. The model is consistent with previously developed in the literature asymptotic theories of the flow and deformation around isolated droplets in the limit of small capillary, Ca , as well as small particle Reynolds, Re , numbers. These asymptotic solutions are also used to uniquely determine all the model parameters, making it the only macroscopic emulsion model that is consistent with all available asymptotic theories for both small Ca and Re numbers. The governing equations are obtained from the Poisson and dissipation brackets, as developed for an incompressible fluid system endowed with an internal contravariant second order tensor, subject to the imposition of the constraint of a unit determinant. First proposed by Maffetone and Minale (*J. Non-Newtonian Fluid Mech.*, vol. 78, 1998 227), this constraint physically corresponds to the conservation of the volume of the dispersed phase in the emulsion. The Hamiltonian of the emulsion is expressed through the surface energy of the dispersed phase, in addition to the kinetic energy, following previous work by Grmela et al. (*J. Non-Newtonian Fluid Mech.*, vol. 212, 2014, 1), but employing a more accurate evaluation of the surface area in terms of the internal contravariant conformation tensor. Most importantly, micro-inertia effects are then introduced by suitably modifying macroscopic model equations derived in the inertialess limit by introducing a new non-affine term that couples the conformation and the vorticity tensors in the evolution equation for the conformation tensor. This derivation and resultant constitutive equation provide a new pathway to rigorously incorporate micro-inertia into general, conformation tensor-based, models for complex fluids. Structural predictions of the ellipsoid droplet morphology obtained with the new model are compared against classic experiments by Torza et al. (*J.*

Colloid Interf. Sci. vol. 38, 1972, 395) and by Raja et al. (J. Fluid Mech. Vol. 646, 2010, 255) showing good agreement.

New rheometric tools for complex materials

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There is a broad range of standard rheological tests which can be used to characterize the rheological behaviour of complex materials. Nevertheless there are still limitations, or parameters which haven't been considered extensively until now. Aim of the contribution is to highlight several new tools which can be of interest for advanced rheological testing and which can help to get profound knowledge of the materials properties.

A rheometer with two drives located on opposite sides of the sample opens new testing opportunities. Using such a setup, combined with a new developed extensional fixture, measurements towards small tensile stresses are possible, since the torque detection is not affected by any mechanical gears or bearings.

A main limitation for characterizing polymer melts and concentrated polymer solutions at large deformations or high shear rates, is known as edge fracture. To limit the impact of edge fracture a cone partitioned plate (CPP) has been recommended [1,2]. By employing a two motor rheometer in a separate motor transducer (SMT) configuration and a newly designed CCP geometry it is possible to measure towards larger strains and strain rates compared to cone-and-plate geometries.

The combination of microscopy with rheological measurements is of interest in order to correlate microstructural properties with the macroscopic rheological behaviour. For such tests rheometers with two drive units working in counter-rotating mode can be of advantage due to the possibility to visualize microstructures kept in the stagnation plane.

A new experimental method for studying the mechano-optical rheology of polymeric liquids and soft matter materials is based on a combination of rotational rheology and a recently developed optical technique - shear-induced polarized light imaging (SIPLI) [3]. The method provides a unique opportunity to monitor a complete sample view during rheological measurements in plate-plate and cone-and-plate geometry. Simultaneous SIPLI and the rheology of the oriented lamellar phase of block copolymers and liquid crystals as well as a direct relation between the shish formation and the polymer melt viscosity upturn during flow-induced crystallization of semi-crystalline polymers are presented. Moreover SIPLI can be used for quantitative birefringence measurements.

While it is already known that ambient condition can have an impact on the rheological properties of materials mostly only the impact of temperature is taken into account during rheological testing. Nevertheless, for some materials also relative humidity of the ambient air can influence the rheological properties. Hence using special accessories to control temperature and relative humidity separately during rheological testing can be of advantage. The presentation will highlight some examples where setting temperature and relative humidity helps to get a better understanding on the materials properties at processing and storage conditions.

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Probing viscoelastic properties of complex fluids by piezo-rheometry in the intermediate frequency range

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We discuss the implementation of a piezo-driven shear cell for a range of soft materials. We perform small amplitude oscillatory rheological tests probing the little explored intermediate frequency range of 20 to 1000 Hz in different Soft matter systems such as linear polymer melts and colloidal glasses.

Commercial rotational Rheometers are very versatile, however in many systems such as polymer solutions, colloidal suspensions and semi-crystalline polymers, the classic approach to reach high frequencies, time-temperature superposition, cannot be applied as temperature alters the thermodynamic state of the system. Piezo-driven rheological measurements have been discussed in the literature. They can enhance the frequency spectrum and address this issue, while at the same time bridging the frequency gap between rheometers and other devices like torsional resonators or indirect experimental techniques such as Diffusive Wave Spectroscopy and Brillouin Light Scattering which provide us insights into very high frequency zone. The low required sample volume, the extensive frequency range, the uniformity in the shear field and the small applied deformation - critical for potentially fragile systems - are among some of the vital characteristics that prove this technique a valuable tool, in probing the linear mechanical response of soft matter systems. We present the technique and its implementation, discuss the various problems and remedies, and apply it to two systems, a glass of hard colloids and an entangled linear polymer solution. In the range 20-1000 Hz, the former exhibits beta relaxation (in-cage rattling) and the latter entanglement network dynamics (fluctuations of strands). Comparison against data obtained with rotational rheometers is very satisfactory and confirms that this is a valuable complementary rheological tool.

Wall slip: a lubricated frictional process?

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In many situations it is observed that yield stress fluids such as foams, emulsions, concentrated suspensions and colloids, glide along smooth solid surfaces, in the sense that the bulk material apparently moves as a rigid block for a stress lower than the yield stress τ_c [1-3]. The basic approach of wall slip consisted to fit a model to the apparent flow curve (shear stress vs velocity) in the slip regime (i.e. for a stress below the yield stress), for the different material classes. Generally power-law dependencies for the stress vs velocity variations were obtained, with an exponent ranging from $\frac{1}{2}$ to 1. Cloitre and Bonnecaze [4] first provided a physical analysis of the process that has the potential to be generalized to any type of jammed systems. This approach relies on the balance between attractive and repulsive forces, due respectively to the osmotic pressure resulting from the repulsive forces between the particles in the bulk and to the lubricated liquid flow along the wall. On the other side Ballesta [5] showed that a linear velocity variation plus a constant stress term well represents their data with hard-sphere colloidal suspensions, but did not observe a clear dependence of the liquid layer thickness on the osmotic pressure.

In an attempt to get a comprehensive understanding of this phenomenon we used various smooth surface types and water-based jammed systems whose structures are expected to cover a wide range of possibilities of element types and interactions: emulsions (jammed droplet network), clay suspensions (flocculated network), Carbopol gel (jammed water blob network), ketchup (concentrated suspension in water), mustard (concentrated suspension in an oil-water mixture), foam (bubble network). We determined the flow properties of each material by a series of creep tests in a wide range of stresses and over a sufficient time to get steady flows. This makes it possible to obtain the usual apparent flow curve with the wall slip regime beyond a critical stress τ_c' and below the material yield stress τ_c . However we show that wall slip takes the form of a viscosity bifurcation process: around τ_c' the apparent shear rate evolves either towards stoppage or to a flow at a shear rate larger than a critical (finite) value. Finally we conclude that the origin of τ_c' is an artefact related to the shearing of the line of contact.

The same trends are observed for a thixotropic material (here clay), which is known to exhibit a viscosity bifurcation around the yield stress (associated with a critical shear rate). Thus wall slip now allows to get steady flows in a wide range of shear rates below this critical shear rate. However the transition from the slip regime to the homogeneous flow exhibits an original trend: if the critical shear rate is sufficiently large there is a jump of shear rate between the wall slip and the homogeneous flow regime, i.e. no steady flow can be obtained in this range of shear rates.

Finally, looking at the velocity vs stress curves for all our materials, it appears that wall slip of all these materials on smooth surfaces follows an affine stress vs velocity law. This law contains a small constant term independent of pressure and a term equal to the stress needed to simply shear the interstitial liquid in a layer of almost constant thickness ($40\pm15\text{ nm}$) for all materials, i.e. independent of structure, concentration and interactions of the elements with the surface. This film thickness might be fixed by the repulsion between particles and solid surface due to the disjunction pressure in the liquid film separating them. Thus wall slip of water-based materials on smooth surfaces appears to follow a universal simple behavior.

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Prediction of long chain branching in uniaxial elongational flow

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In extensional flows, the molecular stress function MSF model can predict the behavior of polymers with two structural parameter: f_{\max} and β . β is defined as the ratio of the total number of segments to that of the backbone. f_{\max} represents the maximum imposed tension to the backbone tube which equally means the minimum tube diameter [1-2]. The strain hardening behavior of LDPE in unidirectional flow is studied by strain control rheometer at different strain rates. The MSF model predictions are presented for low density polyethylene in uniaxial test.

LDPE 0200 was purchased from Bandar Imam petrochemical company, Iran. Dynamic oscillatory shear experiments were performed by Anton Paar UDS 200 130°C. Uniaxial elongational viscosity measurements were performed by ARES G2 at 130 °C with the EVF

fixture. Figure 1 shows the superimposed storage and loss moduli of the LDPE. Dynamic moduli are fitted with 10-element Maxwell model. Figure 2 shows the uniaxial elongational viscosity of LDPE. The MSF model predicts well the experimental data and the strain hardening.

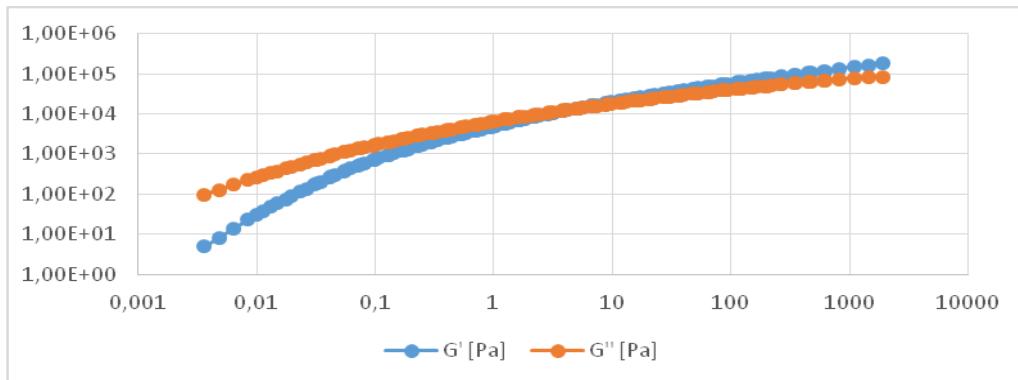


Figure 1. Storage and loss moduli of LDPE at 130°C.

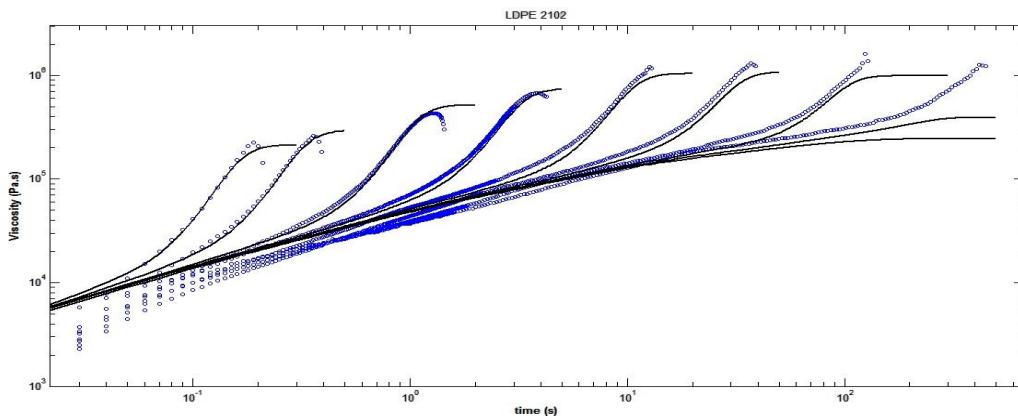


Figure 2. Uniaxial elongational viscosity of LDPE2102 at 130° C

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The dependence of extrudate swell on rheological parameters

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The extrudate swell of an industrial grade high molecular weight high-density polyethylene (HDPE) in capillary dies is studied using the integral K-BKZ constitutive model. The non-linear viscoelastic flow properties of the polymer resin are studied for a broad range of large step shear strains and high shear rates using the cone partitioned plate (CPP) geometry of the stress/strain controlled rotational rheometer. This allowed the determination of the rheological parameters accurately, in particular the damping function, which is proven to be the most important in simulating transient flows such as extrudate swell. A series of simulations performed using the integral K-BKZ Wagner model with different values of the Wagner

exponent n , ranging from $n=0.15$ to 0.5 , demonstrates that the extrudate swell predictions are extremely sensitive to the Wagner damping function exponent. The extrudate swell is also dependent on the β parameter that controls the extensional behavior. Using the correct n and β values resulted in extrudate swell predictions that are in excellent agreement with experimental measurements.

Wall slip and melt fracture of polyisobutylenes

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The rheology and wall slip behavior of several polyisobutylene (PIB) melts with different molecular weights were determined using parallel-plate and capillary rheometry. All PIBs studied were found to slip even at very low shear rates. The transition from weak to strong slip (nearly plug flow) was found to occur at a wall shear stress of approximately 0.078 MPa. The slip model developed by Ebrahimi et al. (*J. Rheol.*, 2015) based on double reptation was used in order to relate the slip velocity, V_s , to the molecular weight distribution of the polymers. It was found for the monodisperse polymers (extracted from the general model) that the slip velocity scales with wall shear stress, σ_w , and the number average molecular weight, M_n as $V_s \propto M_n^{-2} \sigma_w^{1/n}$ with n equal to the local slope of the flow curve of the corresponding polymer, $n \equiv d(\log(\sigma_w)) / d(\log(\dot{\gamma}_w))$. The exponent -2 in the molecular weight dependence for PIBs was found to be the same as previously reported for high-density polyethylenes (HDPEs) and polybutadienes (PBDs), suggesting that it is universal for linear polymers. Their processability of these polyisobutylene (PIB) was also investigated in parallel with wall slip. Direct focus was given on the occurrence of melt fracture phenomena, such as sharkskin and gross melt fracture (GMF). Due to their highly elastic nature, high MW PIBs were found to exhibit gross melt fracture instability even at very low shear rates rendering their processing an impossible task. An increase in temperature resulted in postponing both instabilities (sharkskin and gross) to higher shear rates thus making their processing easier. Finally, decreasing the entrance angle below a critical value resulted in postponing the onset of GMF to higher shear rates.

Attempts to measure shear viscosity and normal stresses in polymer melts

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Progress in polymer physics and processing relies on the development of reliable molecular constitutive equations. The latter relies, in turn, on the availability of reliable experimental information, especially with well-characterized polymers. Concerning shear, flow instabilities such as banding, wall slip and edge fracture represent the main obstacles to the advancement of the field. Recent developments have enabled the measurement of shear viscosity over an unprecedented range of Weissenberg numbers by means of the so-called cone-partitioned plate geometry. However, measurement of N1 and N2 is more challenging. Here, we review the relevant measurement methods and present new efforts to address, at least partially, the challenges. Results with polystyrene melts suggest that relatively easy and reliable measurements of all material functions for melts are possible.

Dynamics of associating star polymers with self-healing performance, studied by rheology and Brownian dynamic simulation

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Self-healing polymeric materials have recently attracted a great deal attention due to their built-in ability to repair physical damage, effectively preventing catastrophic failure and extending the material lifetime. Herein, we present an approach to molecularly control the viscoelasticity and self-healing behavior of polymeric materials that is based on reversible covalent disulfide inter-intra dynamic exchange.

We examine which polymeric architecture would be best-suited for self-healing materials. Since bond formation/ re-formation essentially needs intimate contact of materials, the flow properties of materials should be assessed, in the region where the surfaces of the damaged materials can readily approach a distance close enough for bond re-formation. Taking these requirements into consideration, polymers with a branched architecture, should be more suitable than linear counterparts. The functional groups responsible for healing were introduced at the extremity of the arms, to ensure their accessibility for intermolecular interactions and thus facilitate a rapid self-healing process.

In this work, we study the viscoelastic proprieties of this system using linear and nonlinear shear rheology through the study of the inter-intra stars disulfide exchange dynamics. We analyze the latter behavior within the framework of the rubber elasticity theory. A percentage ranging between 20 to 25 % of active stickers (connecting arms from different stars) is found from simple estimations and Brownian dynamic simulation where the rest of the stickers are allowed to form loops (connecting arms from the same star) or to close among them in one arm, which is in very good agreement with the experimental percentage for the active stickers. Further insight regarding the inter-intra, i.e., active-inactive stickers is gained by means of nonlinear start-up and relaxation tests.

Flow of colloidal gels and attractive glasses. Comparing experiments with computer simulations

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The rheology of non-ergodic states of attractive colloids has been the subject of intense investigation both experimentally and by computer simulations [1,2], while theoretical models aim in describing the dependence of their viscoelastic properties on key parameters such as volume fraction and attraction strength. Here we examine fundamental aspects of the linear and non-linear response of such systems, ranging from low and intermediate volume fraction gels to highly concentrated attractive glasses, and compare experimental findings with Brownian Dynamics simulations results. We mainly focus on the way such systems yield under the application of steady or oscillatory shear via start-up shear tests and large amplitude oscillatory shear, as well as on the mechanisms of gel reformation and accompanied stress relaxation after shear cessation. We discuss the phenomenology of two step yielding, widely observed experimentally, and the underlying mechanisms and relevant length- and time-scales

that cause such behavior and contrast it with findings from computer simulations with and without hydrodynamic interactions.

We further report on the types of rejuvenation protocols, either by shear (steady or oscillatory) or by temperature or volume fraction quench, as a tool to either provide reproducible initial states or, more interestingly, to tune the final properties of such non-equilibrium states (gels or attractive glasses).

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Surfactant destabilisation in thin-film shear flows

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We consider a two-fluid shear flow where the interface between the two fluids is coated with an insoluble surfactant. The flow configuration comprises two superposed layers of viscous and immiscible fluids confined in a long horizontal channel. The two fluids can have in general different densities, viscosities and depths, but here we are interested in the case with one of the layers being very thin compared to the other. We therefore derive an asymptotic model in the thin-layer approximation, consisting of a set of nonlinear PDEs to describe the evolution of the film and interfacial surfactant disturbances. The aim of this study is to investigate the effect of surfactants on the flow stability. Interfacial instabilities are induced due to the acting forces of gravity and inertia, as well as the action of Marangoni forces generated as a result of the dependence of surface tension on the local surfactant concentration. We find that in the inertialess limit, a stably stratified flow can become unstable if an insoluble surfactant is present at the interface. Inertial flows are known to be unstable in the absence of surfactant (due to density and viscosity stratification); yet, we identify regions in parameter space where stability is supported due to the existence of the surfactant monolayer at the interface. The destabilising mechanism related to the Marangoni forces will also be discussed. Future work includes considering the problem with a soluble surfactant that can dissolve into the thin film.

Linear stability of viscoelastic oscillatory shear flow

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Viscoelastic oscillatory shear flows are a fundamentally important class of rheometric flows, and in the present study, we utilize Floquet analysis to examine the linear stability of the flow between two planar harmonically oscillating walls. We focus on ‘highly-elastic’ strongly shear-thinning Giesekus fluids at low Reynolds numbers where Newtonian flows are stable. The choice of flow and fluid parameters is guided by experiments with wormlike micellar solutions in oscillatory pipe flow where instabilities have been observed (Casanellas and Ortín, 2014) (though we do not consider or attempt to model shear banding).

Numerical results indicate that the flow is unstable if 1) the product of the polymer relaxation time and oscillation frequency (De) is large and 2) both the Weissenberg and Strouhal numbers are $\approx O(1)$. The figure below shows the critical Weissenberg number for

the onset of instability as the wall oscillation frequency is varied. There is a clear oscillatory character to the neutral curve which can be connected to the wave-like nature of the background flow. For the flow and fluid parameters of interest, the base state can be thought of as a trapped elastic wave, and for cases where the channel height is an integer multiple of the base-state wavelength, relatively large background shear is generated which enhances the instability and lowers the critical Weissenberg number. Casanellas and Ortín (2014) observed qualitatively similar behavior in their experiments.

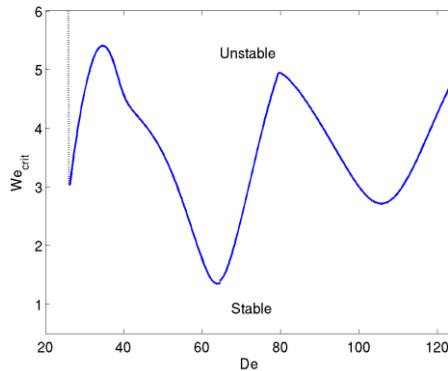


Figure 1: Critical Weissenberg number for Floquet instability of oscillatory shear flow, $Re = 0:025$. Flow regimes corresponding to points above the solid curve and to the right of the dotted line are linearly unstable.

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Weakly-nonlinear interfacial instabilities in two-layer viscoelastic Couette flow

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The stability of two-layer plane Couette flow is a problem of substantial practical interest as it provides insight into the stability of co-extrusion processes. The linear stability of elastic two-layer Couette flow has been extensively studied with Chen [1991] identifying an elastic instability that occurs when the thinner layer is more elastic. Subsequent studies considered similar flows and a range of constitutive models but typically focused on the linear problem.

In this study, we consider the weakly-nonlinear stability of two-layer Couette flow with two Oldroyd-B fluids for the case where one layer is thin. Taking this thin-layer thickness as a small parameter, asymptotic analysis is used to derive a nonlinear evolution equation for the interface height. The influence of the thick layer is felt through a nonlocal coupling term which is obtained by solving a system of linear equations which are a simplified viscoelastic analogue to the Orr-Sommerfeld equation. The evolution equation allows us to clearly identify the influence of the normal stresses at the interface on both the initial instability and the subsequent nonlinear dynamics. Results from numerical simulations illustrate: 1) an array of unsteady states including traveling waves and chaos (figure 1a), 2) competition between elastic instability and instability due to viscosity stratification, and 3) regularizing dispersive effects associated with viscoelasticity in the thick layer (figure 1b). Results from a parallel study on viscoelastic two-layer falling films will be presented as well.

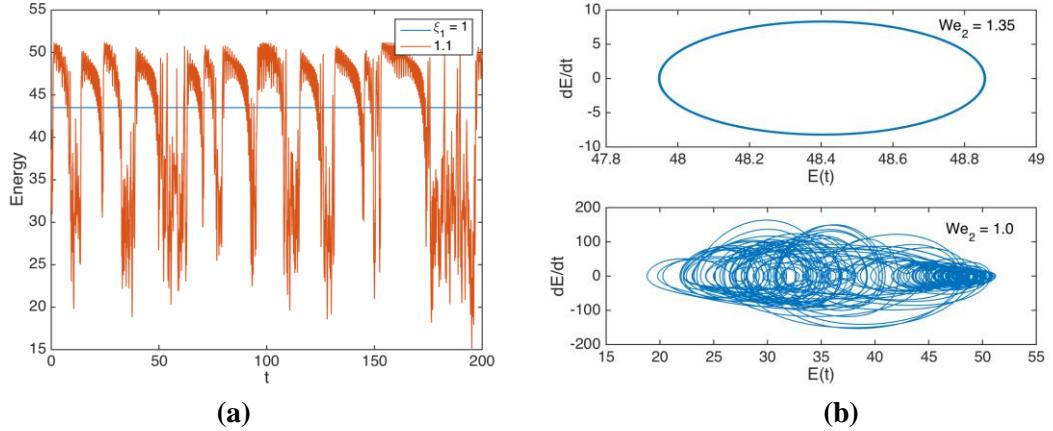


Figure 1: (a) Interfacial energy in inertia-less 2-layer Couette flow. Increasing the Weissenberg number in the thin layer (via the parameter $_1$) results in a transition from simple translating traveling waves to a chaotic state. (b) Phase planes illustrating the regularizing influence of elasticity in the thick layer. The thick-layer Weissenberg number is increased from 1 to 1:35 while the thin-layer elasticity is also increased so that the normal-stress jump at the interface remains the same. The chaotic nonlinear state then transitions to an orderly time-periodic state even though the linear growth rate remains the same.

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Static and dynamic response of coated microbubbles

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Static and dynamic simulations of coated microbubbles are performed subject to step and acoustic pressure disturbances. Bifurcation diagrams are constructed indicating a wide range of possibilities for static equilibrium. It is seen that shell elasticity and viscosity prevent jet formation, by redistributing the energy over a wider portion of the shell. When a nearby wall interacts with an acoustically excited microbubble, growth of buckling modes occurs very fast in a manner that follows the compression only pattern. It is thus seen that acoustic interrogation of lipid shells may introduce dynamic effects that will affect microbubble behavior via a number of shell parameters, such as shell viscosity and bending stiffness, so that shell elasticity modulus cannot be reliably recovered.

When a static interrogation is employed, such as the one involving AFM measurements, due to the hydrophilic nature of lipid shells and the cantilever and the softness of the shell, intermolecular forces are taken into account in the contact area. They are represented by the disjoining pressure between the shell and cantilever mediated by the very thin water film that separates them. As a result, for a large enough value of the interaction potential the solution branch characterized by flattened shells in the contact region is stabilized, and the linear Reissner regime is recovered for a wide range of deformations. Monitoring the slope of the linear regime of AFM measurements of lipid monolayer shells, coupled with the point of departure from linearity provides reliable estimates of shell area dilatation and bending stiffness.

Improved convergence based on linear and non-linear transformations at low and high Weissenberg number

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For a variety of fundamental viscoelastic flow problems, we investigate the accuracy and efficiency of linear and non-linear transformations on the series solutions obtained by asymptotic methods. Well-known differential constitutive equations such as the Upper Convected Maxwell / Oldroyd-B, exponential and linear Phan-Thien and Tanner, Giesekus, and FENE-P models are used. The asymptotic, regular and singular, techniques are performed at both the Newtonian (zero Weissenberg number) and the purely elastic limits (infinite Weissenberg number). In all cases, the radius of convergence of the transformed solutions increases substantially compared to the original series solutions. By combining the transformed solutions from both limits and comparing with the exact (analytical, semi-analytical, or numerical) solutions, excellent agreement over the entire range of the Weissenberg number is demonstrated. The results show that, contrary to intuition, viscoelastic phenomena at Weissenberg number of order unity can be predicted accurately. Based on the analysis and conclusions of the present work, a simple solution strategy of the governing equations for more complicated viscoelastic flow problems is proposed.

Structural processes in elastoviscoplastic materials

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Constitutive modeling of elastoviscoplastic materials has drawn a lot of attention in the literature. A recent comparison of EVP constitutive models has been conducted by Fragedakis et al. (2016), where it was concluded that the proposed model by Saramito (2007, 2009) was overall superior among others in predicting accurately the behavior of yield-stress materials when elasticity is also taken into account. In the present work, we attempt to refine this model by incorporating the Isotropic and Kinematic Hardening mechanisms, as discussed in Dimitriou & McKinley (2013, 2014). The newly proposed SRM-IKH model is expressed in a tensorial form, along with the equations describing the structural evolution of the material. Initially, in order to grasp the physical aspects of the aforementioned hardening mechanisms, we explore the differences between the various model predictions and explain how the SRM-IKH model can be considered as a generalization of the SRM model. Several prototype flows are considered, e.g. simple shear between parallel plates. The significance of Isotropic and Kinematic Hardening is found to be profound, when studying Large Amplitude Oscillatory Shear with imposed Strain (LAOStrain), since the parameters associated with those mechanisms lead to unique periodic solutions. Next, the problem of the flow between coaxial cylinders is tackled in order to reveal how the hardening mechanisms affect the evolution of solidification boundary. Additionally, the heterogeneity of the stress distribution is examined. The proposed SRM-IKH model is validated by comparing it to the experimental observations by Lacaze et al. (2015). Another issue that is addressed in materials, which exhibit elasto-visco-plastic behavior is multiplicity of the steady state solutions in Taylor – Couette flows, Cheddadi et al. (2012), which is remedied when kinematic hardening is introduced. Finally, unsteady simulations based on the Taylor – Couette flow are considered in order to investigate the contribution of the aforementioned hardening mechanisms on the response of the material due to oscillatory forcing.

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Squeeze axisymmetric flow of a viscoplastic Bingham medium

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We develop an asymptotic solution for the axisymmetric squeeze flow of a viscoplastic medium. The standard lubrication-style expansions of the problem predict plug speed which varies slowly in the principal flow direction. This variation implies that the plug region cannot be truly unyielded. Our solution shows that this region is a pseudo-plug region in which the leading order equation predicts a plug, but really it is weakly yielded at higher order. We follow the asymptotic technique suggested earlier by Balmforth and Craster (1999) and Frigaard and Ryan (2004).The asymptotic solution has the following structure. First, close to the discs there will exist a yielded region, which is a shear flow. Second, in the region surrounding the central plane there is a pseudo-plug region in which extensional strain rates are present. The yield criterion is reached in the pseudo-plug flow zone and exceeded in the shear flow zone. These solutions are joined at the position of the pseudo-yield surface. The obtained analytical expression for the squeeze force is in a good agreement with the previous numerical results of Smyrnaios and Tsamopoulos (2001) and Matsoukas and Mitsoulis (2003). The axisymmetric squeeze flow of a Bingham fluid with slip yield boundary condition at the wall is considered. We provide a asymptotic solution for this type of flow. Depending on the ratio of two dimensionless parameters partial slip (stick-slip) or full slip at the wall (slip) are possible.

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Rheological considerations for modelling of submarine mass failure processes at the Rockall Bank

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The post-failure stage of submarine landslides can be well described by fluid mechanics principles and is often considered as the most significant for tsunami generation. Depending on the selection of the input parameters for the calculation of the shear retarding stress, the flow properties may vary corresponding to different fluid types. Above all, the sediment concentration of the landslide plays an important role on the rheological behaviour. Bingham, Herschel-Bulkley and bilinear fluids are commonly used to represent the rheology of mudflows or muddy debris flows. On the other hand, frictional flow models are often used to study terrestrial and sand-rich flows where there is a lot of grain-to-grain interaction. However, the values of the input parameters are not always known with certainty. In the absence of adequate input data, a common practice in the numerical modelling of submarine sliding is to match the depositional lobes resulting from the simulations, with the landslide deposits observed in the field. In the present work, we use three types of models to compute the total retarding stress and simulate submarine failure at the Rockall Bank Slide Complex, in the NE Atlantic Ocean. The Bingham and the frictional rheology are used to simulate the flow behaviour. The scope of this approach is to understand the effect of the two classical laws in the landslide kinematics. Furthermore, a rheological model that combines the two regimes is also used. To incorporate the hydrodynamic drag, the Voellmy model is employed. The results are validated against the field observations. The effect of the models on the landslide kinematics and final deposition are discussed.

Numerical prediction of the rheological properties of fresh selfcompacting concrete

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Self-Compacting Concrete (SCC) is a high-performance construction material that can simplify classical handling on concrete construction by avoiding the need for additional vibrational compaction. Challenges in the use of SCC lie in ensuring optimal operation of the material in terms of properly filled castings in presence of complex reinforcement arrangements, reduction of entrained gas bubbles and limitation of aggregate separation. A major factor influencing the aforementioned aspects is the rheological properties of SCC mixtures under varying conditions (e.g. content composition, mechanical impact, temperature, moisture). This contribution aims at unified constitutive modelling of SCC in the setting stage. Concrete setting describes the transition from fluid-like fresh concrete, which -in presence of timedeependent transport-reaction processes- develops a porous cementitious structure, to hardened concrete showing solid-like behaviour. The constitutive model is implemented using the open-source finite element framework FENICS and applied to a number of benchmark problems.

Flow in a fluid damper: investigation of the effects of shear thinning and viscoelasticity through numerical simulations

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We present the results of simulations, performed with a finite volume method, of the flow inside a fluid damper during its operation. The operation of such a damper is based on the dissipation of mechanical energy by the reciprocating axial motion of a shaft equipped with a piston inside a cylinder filled with a fluid. In the literature, full simulations of the flow inside a damper are lacking, and in most studies the damper is treated as a “black box” with only the overall response recorded and modelled. The fluid employed is commonly silicon oil (polydimethylsiloxane), which exhibits both shear-thinning and viscoelasticity. Therefore, for a given damper configuration, we performed simulations assuming that the fluid obeys the Newtonian, Carreau-Yasuda, and simplified Phan-Thien – Tanner (PTT) constitutive equations, respectively. The damper response (reaction force) to a sinusoidal input (shaft displacement) is recorded for various excitation frequencies. Comparison between the Newtonian and Carreau-Yasuda responses reveals the effect of shear-thinning, while comparison between the Carreau-Yasuda and PTT responses reveals the effect of elasticity. The “signature” of Newtonian flow is that the force is proportional to the instantaneous shaft velocity. Shear thinning, on the other hand, flattens the force / displacement or velocity graphs, as the lowering of the viscosity at higher shear rates attenuates the force rise. At high frequencies, shear thinning may be such that inertia effects may become important, in which case hysteresis is introduced in the force-velocity graph, causing greater forces during the acceleration phase of the shaft than during the deceleration phase. Elasticity is also manifested through the introduction of hysteresis, but in the opposite sense than inertia.

Analysis of pressure-driven flow in long channels of a Herschel-Bulkley fluid with pressure-dependent rheological parameters

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The lubrication flow of a Herschel-Bulkley fluid in a symmetric long channel of varying width, $2h(x)$, is modeled extending the approach proposed by Fusi et al. (J. non-Newtonian Fluid Mech. 221, 66-75, 2015) for a Bingham plastic. Moreover, both the consistency index and the yield stress are assumed to be pressure-dependent. Under the lubrication approximation the semi-width of the unyielded core is found to be given by $\sigma(x) = -(1+n/h(x)) + C$, where n is the power-law exponent and the constant C depends on the Bingham number and the consistency-index and yield-stress growth numbers. Hence, in a channel of constant width, the width of the unyielded core is also constant, despite the pressure dependence of the yield stress, while the pressure distribution is not affected by the yield-stress function. With the present model, the pressure is calculated numerically solving an integro-differential equation and then the position of the yield surface and the two velocity components are computed using analytical expressions. Some analytical solutions are also derived for flat and linearly varying channels. The lubrication solutions are also on different other geometries and their advantages and limitations are discussed. The implications of the pressure-dependence of the material parameters are also investigated.

The lock-on regime in the wake of a periodically perturbed flow of a viscoplastic fluid past a confined circular cylinder

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This research outlines the extension to viscoplastic fluids of one of the classical problems in fluid dynamics, namely the case of periodically perturbed flow over a circular cylinder in confined geometries. It is well known that in the Newtonian case 2D vortex shedding appears for Reynolds numbers between 50 and 106, depending on fluid properties and flow configuration. While the vortex shedding phenomenon takes place, periodic forces are exerted on the cylinder surface. The lift force has the same frequency as the vortex shedding cycle, while the frequency of the drag force is twice the shedding frequency. When the cylinder oscillated, with a periodic motion normal or parallel to the incident flow, the phenomenon can be dramatically altered. Furthermore, by varying the amplitude and frequency of oscillation, the phenomenon can be controlled. One of the most interesting characteristics of the interaction between the oscillating cylinder and the flow is the lock-on phenomenon, where the oscillation frequency and shedding frequency are synchronized. This also appears when the near wake of a circular cylinder is subjected to an incident mean flow with periodic velocity perturbations, the case that we consider in the present work.

We consider the case of an incompressible flow past a confined cylinder, where the incident mean flow is subjected to periodic velocity perturbations. Numerical simulations are conducted at a fixed Reynolds number of $Re=100$, based on the cylinder diameter d and the mean fluid velocity \bar{u} . The amplitude of the periodic velocity perturbation is $\Delta u / \bar{u} = 0.10, 0.20, 0.25, 0.30$. The frequency ratio is varied from $f_\theta / f_0 = 1.4$ to 2.3, where f_0 is the natural Strouhal frequency in the unforced (unperturbed) wake and f_θ is the perturbation frequency. Bingham numbers (Bn) in the range $Bn=0$ to 0.5 are considered.

Figure 1 shows the lock-on regime in terms of the frequency ratio f_θ / f_0 and the dimensionless amplitude $\varepsilon = \Delta u / (2\pi f_0 d)$, where Δu is the amplitude of the flow perturbations. Preliminary results for the lock-on regime from the current simulations at $Bn=0$ (Newtonian fluid) are consistent with the literature. Viscoplastic results ($Bn > 0$) will be reported at the conference.

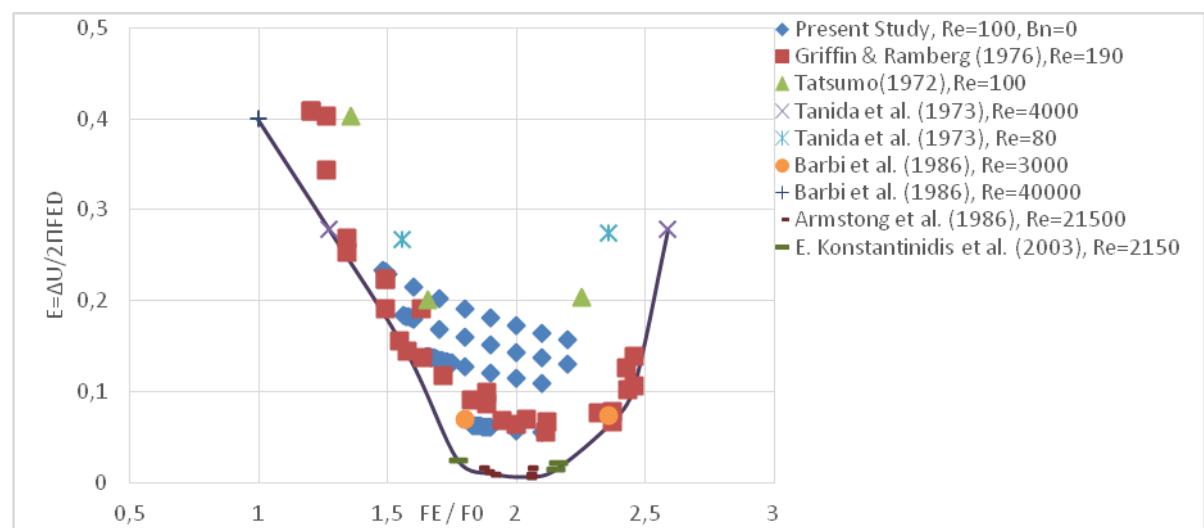


Figure 1

POSTERS

Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics

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In the constitutive modelling of polymer flows, convective constraint release (CCR) is the mechanism accounting for a variable entanglement density as entanglements or topological constraints are continuously destroyed and regenerated due to applied flow, even at moderate shear rates. Atomistic non-equilibrium molecular dynamics (NEMD) simulations of entangled polyethylene melts provide direct evidence for a decrease in the average number of entanglements per chain in the melt with increasing shear rate [1]. Motivated by this, Marrucci and Ianniruberto [2] proposed a new version of the CCR theory for polymer flows by considering (in addition to the evolution equation for tube orientation and chain stretch) an extra equation for the (scaled) entanglement density.

In the present work, we revisit a recently proposed constitutive model for the rheological description of entangled polymer melts developed in the context of nonequilibrium thermodynamics [3] by allowing for a variable entanglement density due to applied flow. To this, we have added the entanglement density to the vector of state variables and have properly redefined the Poisson and dissipation brackets, as well as the expression for the free energy of the melt. We anticipate the new constitutive model to be able to describe rheological data for the flow behaviour of entangled polymer melts using a smaller value of the CCR parameter than the model with a constant entanglement density. Using the new model to describe available rheological data is part of ongoing research work.

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Confined viscoplastic flows with heterogeneous wall slip

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The steady, pressure-driven flow of a Herschel-Bulkley fluid in a microchannel is considered assuming that different power-law slip equations apply at the two walls due to slip heterogeneities, allowing the velocity profile to be asymmetric. The different flow regimes are identified and comparisons with available experimental data on soft glassy suspensions are made. These results open new routes to manipulate the flow of viscoplastic materials in applications by controlling the topography and chemistry of the wall surfaces.

Surface tension driven microfluidic blood flow: red blood cell aggregation and viscosity effects

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Microfluidic applications for blood diagnostics are increasingly popular due to various advantages they offer. The perfusion of the fluid in such devices is achieved in general using pressure driven set-ups. Surface tension driven blood flows is another option and various studies in the literature examine the behaviour of blood in such microfluidic flows. However, the majority of these studies have not examine the influence of the red blood aggregation phenomenon, which dominates the non-Newtonian nature of blood. In the present study, we examine the influence of the red blood cell aggregation phenomenon in surface tension driven flows in a rectangular microchannel. Non-aggregating and aggregating blood samples are tested and the flow characteristics in the microchannel are analysed, through micro-PIV based techniques. The intensity of aggregation is estimated using previously developed algorithms and the effective viscosity of the samples in the device is analysed using theory on surface tension driven flows and blood constitutive equations. Preliminary analysis show that the non-Newtonian nature of blood has an impact in the flow characteristics.

Shape effects on the rheological behavior of polymer-grafted nanoparticles in solution

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The large majority of rheological investigations with soft colloids involve spherical particles. However, in several applications the particles are anisotropic. Here, we focus our attention on polymer-grafted nanoparticles in solution and compare three soft systems with the same chemistry, similar grafting density, same number of monomers per grafted arm but different core shape (spheres, cylinders and lamellas). Solutions in the dense regime at the same mass concentration have been investigated by means of light scattering and rheology in both linear and nonlinear regime. We find that, at the same weight concentration the shape affects substantially the relaxation times, yielding mechanisms and residual stresses, which reflect different particles arrangement in solution. We compare against relevant data in the literature with hard spheres, ellipsoids and other soft spheres, and attempt at extracting a generic phenomenological picture of rheology vs. shape and concentration.

On the tails of probability density functions in Newtonian and viscoelastic turbulent channel flows

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Direct numerical simulations (DNS) of Newtonian and viscoelastic turbulent channel flows generate crucial data to analyze and understand the nature of turbulence modification by

viscoelasticity---see, for example, [1] for a recent review. Such an understanding is necessary to enable better drag reduction technologies. Previously, we have shown how viscoelasticity can significantly alter the non-normal character of the probability distributions (PDFs) of many of the turbulent statistics in the flow [2]. In this work, we report another characteristic of those PDFs for the velocity and its derivatives in Newtonian and viscoelastic turbulent channel flows. More specifically, we report the power law index of their tails, as obtained by applying Hill's estimator. We have also used statistical methods to guide as for the evaluation of the results [3]. In particular, fat (or heavy) tails corresponding to an asymptotic power law behavior with low power law exponents have been observed in the PDFs for both Newtonian and viscoelastic cases. In many instances, the power law index is small enough to imply infinite fourth, or even third, moments. We also show that viscoelasticity leads to PDFs with fatter tails than the Newtonian ones. This finding explains why viscoelastic turbulent DNS are much more demanding computationally than Newtonian ones, requiring for proper resolution of the turbulence statistics much longer times and larger computational domain sizes.

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Multi-scale modelling of high-MW polymer melt viscoelasticity starting from the atomistic level

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At the heart of the very successful reptation theory for the description of entangled polymer melt dynamics is the concept of the primitive path (PP), namely of the shortest path that connects the two ends of the chain (considered as fixed in space) without violating any topological constraints along the chain. From this, one can in principle obtain all linear viscoelastic (LVE) properties of a polymer melt in a rather straightforward manner. Guided from this, we have designed and implemented a computational approach that allows one to obtain the LVE properties of a high-MW polymer melt starting from detailed atomistic simulations for a given polymer chemistry and polymer architecture [1-3]. Our work contains the following steps: 1) We first map atomistic trajectories from the atomistic MD simulations onto trajectories of PPs for moderately entangled polymers of the given chemistry. The latter are used to compute the PP segment survival probability function $\psi(s,t)$ for moderately entangled melts of the given polymer chemistry. 2) The computed curves are used next to parameterize a reliable tube model for polymer dynamics on the basis of the reptation theory, accounting for constraint release (CR) and contour length fluctuation (CLF) mechanisms [4]. The comparison suggests changes to the functional form of the model or to its boundary conditions. 3) The refined tube model is finally employed to predict the LVE properties of the same polymer chemistry but of significantly higher MW [5-6]. We will present results from such a hierarchical computational approach for the cases of a mono- and bi-disperse cis-1,4-

polybutadiene melt. A detailed comparison with independently measured experimental data available in the literature for the MW dependence of the zero-shear viscosity and the functions $G'(\omega)$ and $G''(\omega)$ of this polymer will also be presented.

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Analytical expressions for the velocity field of polymeric fluids and polyelectrolyte in microchannels.

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The understanding of the unexpected phenomena (e.g. the reduction of drag of force with the increase of viscoelasticity) that occur when polymeric fluids flow through channels in microscale plays important role in technological areas^[1]. All these phenomena are related with the cross-stream migration of the polymer. In this work, analytical expressions for the velocity field and the stress tensor in channel geometry under steady state flow conditions are derived. Two phases^[2] are assumed, one polymeric with a solvent contribution^[3] and the other consisting of pure solvent which represents the depletion layer. To account for the viscoelastic nature of the flexible macromolecules, the use of viscoelastic constitutive differential models for stresses is obligatory. The FENE-P model is preferred because it is derived from the kinetic theory for finitely extensible non-linear elastic dumbbells with a Peterlin approximation for the average spring force and can capture the pronounced shear-thinning that these systems exhibit^[4]. Additional tests with the PTT model are conducted^{[5], [6]}. Next, a polyelectrolyte solution is examined by adding an electrophoretic force^[7]. Here, the Debye-Hückel linear approximation is proposed for the calculation of the electric charge density^[8]. After deriving the equations governing the velocity profiles, comparison is made with experimental data^[9].

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Using new magnetic rheological fluids in automobiles suspension systems- Comparison study

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Recently, the so-called magneto-rheological (MR) fluids usage as a shock absorbers' fluid has been increasing. Many types of devices have been designed to implement this versatile fluid, including linear dampers, clutches, work-piece fixtures, and polishing machines. Such devices have been used in automobiles, washing machines, bicycles, prosthetic limbs, and even smart structures. This paper presents the usage of MR fluids in automobile suspension system; a comparison is presented here between the traditional fluids and the MR fluids including its performance and efficiency.

Rheological investigations on dynamic covalent four-armed star poly(ethylene glycol) model hydrogels

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Dynamic covalent polymeric networks have attracted the attention of the scientific community in the last ten years due to their ability to self-heal and expand their service life [1,2]. The self-healing ability arises from the presence of reversible dynamic covalent bonds, which serve as cross-links between the polymeric chains. Among them, the acylhydrazone reversible dynamic covalent bond can be formed by the reaction between an acylhydrazide and a benzaldehyde group [3]. The continuous dissociation and formation of these bonds, under the appropriate conditions, causes a continuous de-cross-linking and cross-linking of the polymeric chains, leading to the self-healing of the network [4]. In this work, we prepared dynamic covalent polymeric networks based on the reversible acylhydrazone bond, by mixing two ethylene glycol homopolymer stars, the one having four terminal benzaldehyde groups and the other one having four terminal acylhydrazide groups [5]. We employed dynamic rheological measurements to determine the formation time for the networks, and to explore their viscoelastic properties at various pH values. Furthermore, we performed frequency-dependent oscillation rheology to estimate the lifetime of the reversible acylhydrazone cross-links, which can be related to the self-healing speed of these dynamic covalent networks.

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Squeeze flow of thixotropic semisolid slurries

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The motivation of this work derives from our interest in the existing and continuously developing technology of processing metal slurries in their semisolid state for the production of consistently high integrity parts. This technology, known also as thixoforming process, implies that the material behaves as a solid when the applied stress lies below the yield stress. Once the yield stress is exceeded, the material behaves either as a shear-thickening or as shear-thinning fluid with a non-linear stress-strain relationship [1-3].

An important issue for the commercialization of the semi-solid process in the production of complex components is the availability of accurate mathematical and computational tools that could describe both the rheological behavior and the material characteristics of the suspension, which are strongly affected from its internal structure and its evolution during deformation. In contrast to other thixotropic materials, semisolid slurries show partially irreversible rheological properties due to the breakage of the welded bonds between the particles [3, 4].

In this work we modeled numerically the classical squeeze flow experiment by including the effects of thixotropy and simulated the compression flow of semi-solid material, when it is compressed from its topside either under constant load or constant velocity, while the bottom side remains fixed [3, 5].

More specifically a structural viscoplastic model based on the Bingham-plastic constitutive equation is proposed. 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.

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Synthesis and characterization of acrylamide-based dynamic covalent amphiphilic polymeric conetworks cross-linked via alkoxime bonds

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Polymer networks possess important properties that make them appropriate for use as materials in various fields for applications in technology and medicine. Most of these networks are prepared using conventional free radical polymerization, leading to materials with poorly-defined structure. Although synthetically more demanding than free radical polymerization, controlled / “living” polymerization results in better-defined polymer networks. This work employs such a controlled radical polymerization method, namely reversible addition-fragmentation chain-transfer (RAFT) polymerization, for the preparation of well-defined dynamic covalent amphiphilic polymeric conetworks (dcAPCN). The constituting linear segments of the dcAPCNs were based on the hydrophilic monomer *N,N*-dimethylacrylamide (DMAAm) and the hydrophobic monomer *N*-laurylacrylamide/*N*-dodecylacrylamide (LauAAm), as well as the monomers 4-formylphenylacrylate (4-FPA) and the phthalimide-protected *O*-(4-vinylbenzyl) hydroxylamine (VBA-P). In all these polymers, the hydrophilic DMAAm block was formed first, kept at a constant degree of polymerization (DP), whereas the hydrophobic LauAAm block was prepared next and at varying DPs. The 4-FPA and VBA-P monomers were polymerized to short segments, corresponding to 5 mol% of the total number of monomer (DMAAm plus LauAAm) repeating units of the linear chain, and serving as cross-linking sites, given their mutual reactivity. After their preparation and characterization of their molecular weights and compositions using gel permeation chromatography and ¹H NMR spectroscopy, respectively, the linear amphiphilic block copolymers were dissolved separately, and the resulting solutions were subsequently mixed in equal portions for the formation of the alkoxime cross-linking bonds and, consequently, the dcAPCNs. Finally, the dcAPCNs were characterized in terms of their dynamic and loss moduli, and gel formation times, using rheology, and in terms of their mechanical strength (stress and strain at break, low-strain Young’s modulus) using compression testing.

Physical separation of colloidal systems

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Small scale fluid dynamics is fundamental to the theory of colloids. In consumer products, a crucial requirement is that the suspended colloids must not settle noticeably during the product’s shelf-life for it to remain effective and convey quality to the consumer.

This combined experimental and modelling study has investigated the phase separation behaviour of colloidal suspensions. An existing settling model uses an empirical equation to control separation, considering gravitational effects and Brownian motion of the particles [1]. This model has been further developed to take into account additional effects, including rheological and chemical influences, within the framework of a convection-diffusion equation. In particular, the model avoids the commonly used hard-sphere assumption, thus taking into account the influence of the ionic double layer which forms on the colloidal particles when dispersed in water. The settling model has been implemented numerically in MATLAB, using a finite difference solver with an adaptive spatial mesh and time-stepping scheme for improved efficiency. Further, a model for the aggregation of the colloidal particles, which may occur depending upon various chemical parameters, has been

investigated both theoretically and experimentally [2]. Aggregation is implemented in the settling calculation via the viscosity model.

The settling model has been shown to compare favourably with highly controlled experiments conducted for different dispersed phase volume fractions and electrolyte concentrations. Indeed, the settling behaviour of silica-water suspensions has been examined by tracking the evolution of the interface which develops between the suspension and supernatant. These experiments have been conducted at both Earth and enhanced gravity, the latter with an analytical centrifuge, using an innovative method for converting the results to Earth gravity conditions.

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Experimental analysis of nanoparticles binding through laminar flow between parallel plates

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Drug delivery systems introduce a new way of treatment and diagnosis in many human deceases like cancer and atherosclerosis, using smart drug carriers to recognize specific biological targets. Nanoparticles surface can be decorated with ligand molecules, transported through the blood, interact and bind specifically on receptor molecules that are over expressed at the diseased cell membrane. In this study, the binding dynamics of spherical particles has been analysed in a parallel plate flow chamber within a laminar flow, mimicking the hydrodynamic conditions in the microcirculation at different physiologically relevant shear rates, S . The effect of particle diameter has been investigated on the non specific binding of microparticles (1.70, 3.43 and 5.33 μm) and the enhancement of binding efficacy using Folic Acid (FA) ligand-receptor mechanism on the specific binding of nanoparticles. Simple scaling laws have been derived showing that the number n of adhered particles for the 1.70 μm , 3.43 μm and 5.33 μm particles scales as $32.6 \cdot S^{-0.733}$, $357.7 \cdot S^{-1.175}$ and $827.6 S^{-1.301}$, respectively. It was observed that increasing the shear rate value of the flow, the number of adhered particles declined and the binding efficiency of microspheres increased with increasing particle size. Concerning nanoparticles specific binding, the presence of Folic Acid (FA) ligands optimally recognised the target cells and enhanced the binding efficiency by an average of 10 times compared with the case of the absence of the targeting agent. The results of our study are of importance in the design of particles that intend to be used for the systemic delivery of drugs or in biomedical imaging.

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