Talk titles and abstracts

Azahar, Adila Aida (University of Leeds)

Numerical modelling of polymer blends using openfoam

We will present numerical simulations of contraction flows of polymer blends using a recently developed constitutive model for polymer blends that incorporates the effects of nonlinear coupling between chains of different lengths. Industrial polymers are typically blended from molecules of different molecular weights. The rheology of such blends is usually modelled as a linear superposition of modes with different relaxation times, for example multimode versions of the Rolie-Poly model. However, this approach neglects the effects of interactions between different length polymer chains. Recently, Boudara (2017) developed a constitutive model for bi-disperse polymer blends based on the Rolie-Poly constitutive equation but using double reptation to incorporate the interactions between short and long chain polymers.

The numerical model is developed within OpenFOAM using the rheoTool package (Pimenta & Alves, 2017), which allows different viscoelastic constitutive laws to be implemented. We have extended rheoTool to include both the original Rolie-Poly model and the coupled-mode blend model of Boudara.

Simulations are carried out for a 2D hyperbolic contraction geometry for both the multimode Rolie-Poly model and the coupled-mode blend model. The effects on the flow and polymer stress of varying the contraction dimensions in both the length and the contraction ratio are explored. In particular we examine how the stretch of the long chain fraction is affected by the blend composition. We are currently extending the work to the full 3D geometry to examine the effect of side walls on the flow.

REFERENCES

Boudara, V. A. H. (2017). Supramolecular and entangled polymer materials: rheological models (Doctoral dissertation, University of Leeds).

Pimenta, F., & Alves, M. A. (2017). Stabilization of an open-source finite-volume solver for viscoelastic fluid flows. Journal of Non-Newtonian Fluid Mechanics, 239, 85-104.

Behra, Juliette (University of Leeds)

The effect of ultrasonication on the rheology, structure and dynamics of Sodium Carboxymethyl Cellulose (Na CMC) solutions

Juliette S Behra, Timothy N Hunter, Olivier J Cayre and Johan Mattsson,(all University of Leeds)

Sodium Carboxymethyl Cellulose (Na CMC) is used for its thickening and swelling properties in a wide range of applications including pharmaceutical, food, home and personal care products, as well as in paper, water treatment and mineral processing industries. However, despite its broad industrial use, Na CMC structure-property relationships in solution are known to be highly complex and influenced by a number of parameters. The focus of this study was to expand fundamental understanding of Na CMC solution structure-property relationship using sonication. The rheological behaviour of sonicated and non-sonicated solutions was characterised and correlated to solution structure and dynamics probed by Static and Dynamic Light Scattering (SLS and DLS), respectively; complementary Size Exclusion Chromatography (SEC) was also performed.

We demonstrate that sonication leads to a decrease in the solution viscosity and a reduced shear-thinning behaviour. Also, the characteristic relaxation time of the slower of the two main relaxation modes observed using DLS was also found to decrease, which is consistent with a correlation between viscosity and this ‘slow’ relaxation mode established in a recent study [1]. In contrast, no qualitative change in the structure upon sonication was observed in SLS experiments. Moreover, both light scattering and SEC measurements suggests that no significant degree of Na CMC chain breakage is caused by sonication and we thus suggest a sonication-induced change in the chain participation of the domains causing the slow mode in DLS. Importantly, over a time-scale of a month after sonication, we observed either a partial or full recovery of the characteristic time of the 'slow' relaxation mode. Also, sonication had no effect on solutions with added salt, suggesting that electrostatic forces are important in explaining the observed effects. Our results will be discussed with reference to models and results published in the literature on similar systems.

[1] Behra, J. S.; Mattsson, J.; Cayre, O. J.; Robles, E. S. J.; Tang, H.; Hunter, T. N. Characterization of Sodium Carboxymethyl Cellulose (Na CMC) aqueous solutions using rheology and light scattering. Submitted to ACS Applied Polymer Materials on October 15th 2018 (Manuscript ID: ap-2018-00022m).

Bin Mohamad, Muhammad Sofwan (University of Edinburgh)
Shape oscillation of free-falling liquid gallium droplet

The dynamics of free-falling liquid gallium droplets in water under the action of gravity were investigated experimentally with high-speed imaging in this study. The frequencies and amplitudes of oscillations of droplets with spherical volume-equivalent diameters ranging from 2.67 to 5.56 mm were deduced. The effect of viscosity ratio to the transient droplet shape was studied by changing the temperature of the liquids in the experiment in the range of 30 to 70°C. The initial shape of the droplets after detachment were found to be prolate-spheroid. Prolate-oblate oscillation began directly after the detachment of the droplet prior to dampening of the liquid-metal into final shape of an oblate-spheroid. The oscillation frequencies were sensitive to the droplets' size rather than viscosity ratio.

Boudara, Victor (University of Leeds)
Nonlinear rheology of entangled, polydisperse linear polymers: the Rolie-Double-Poly model

Whilst there has been much success in modelling the rheology of monodisperse entangled linear polymers, industrial polymers are typically polydisperse with a broad range of molecular weight. A molecular-based constitutive model suitable for polydiperse entangled polymer melts is still lacking.

I will present a simplified tube model for such polydisperse polymers, based on the Rolie-Poly constitutive equation [Likhtman et al. J. NonNewton. Fluid Mech. 114, 1–12 (2003)], that aims at predicting nonlinear rheology, whilst being consistent with the "double reptation" theory in linear rheology. This model extends but strongly simplifies the Read et al. model [Read et al. J. Rheol. 56, 823–873 (2012)] that successfully describes nonlinear rheology experiments on bidisperse blends.

First, I will briefly present the double reptation theory, then detail the simplified model in case of a bidisperse blend, before generalizing to the polydisperse case. Then, I will discuss the apparent enhanced stretch relaxation time that emerges naturally from the model in the bidisperse blend case, and show that our model is in qualitative, and largely quantitative, agreement with experimental data on both bidisperse and polydisperse melts.

Finally, I will present a new rheology software, RepTate, where that new theory is implemented, and provide an example of usage.

Capobianchi, Paolo (University of Strathclyde)
Thermocapillary motion of a Newtonian drop in a dilute viscoelastic fluid

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The thermocapillary motion of a deformable Newtonian droplet in an viscoelastic fluid matrix is numerically investigated under the assumptions of negligible momentum and thermal convection. An initially quiescent droplet is released in a three-dimensional box-shaped domain and put in motion under the effect of the thermocapillary stresses arising at the droplet interface generated by the presence of an imposed linear temperature distribution. The problem is formulated under the framework of a hybrid level-set volume of fluid approach and solved using an adaptive mesh strategy. The departures from the Newtonian behaviour are quantified via the “thermal” Deborah number, DeT, and are accounted for by adopting either the Oldroyd-B model, for relatively small DeT, or the FENE-CR constitutive law for a larger range of DeT. In addition, the effects of model parameters, such as the concentration c (or equivalently the viscoelastic viscosity ratio, β), or the extensibility parameter, L2 have been studied numerically using a hybrid volume of fluid-level set method. The numerical results show that the steady-state droplet velocity behaves as a monotonically decreasing function of DeT, whilst its shape deforms prolately. For increasing values of DeT, the viscoelastic stresses show the tendency to be concentrated near the rear stagnation point, contributing to an increase in the local interface curvature.

Cooper, Laura (University of Warwick)
Modelling unsteady viscoelastic flow

Flows through microfluidic networks generally occur at low Reynolds' number due to the small length scales involved. This means that the viscous effects dominate, and the flow is not expected to vary over time. However, viscoelastic fluids display time-dependent behaviour above a critical Weissenburg number, i.e. when the elastic forces are large enough. We investigate the time dependent flow of viscoelastic fluids through periodic microfluidic geometries using computational modelling. The Oldroyd-B and FENE-P constitutive equations are implemented in Comsol Multiphysics, a commercial finite element software, and used to investigate the onset of unsteady flow behaviour in different geometries. The aim is to understand how unsteady viscoelastic flow can be used to enhance various processes, including enhanced oil recovery and heat transfer.

Cox, Simon (Aberystwyth University)
A numerical method for simulating the dynamics of incompressible two-dimensional foams

There is much to be learned about the rheological response of foams and emulsions from a two-dimensional (2D) situation, such as when the bubbles or drops are confined between flat, parallel, glass plates. Major advances in understanding have been triggered by experiments, theory and simulations in 2D (Cantat et al., "Foams: Structure and Dynamics", Oxford University Press, 2013).
The usual mathematical idealization of a 2D foam treats the bubbles either as polygons that fill space without gaps or overlaps (a "dry foam") or as discs (a "wet foam"). Most real foams lie somewhere between these two limits.

This work describes a simulation method that is able to predict the rheology of 2D foams with intermediate liquid fraction while retaining an accurate representation of the bubble shape. It incorporates surface tension forces on the bubble interfaces, and it can account for variations in surface tension due to stretching of the interfaces. Bubble pressures are determined by assuming that the foam is incompressible. In keeping with the 2D nature of the approximation, dissipative forces arise from friction with the bounding glass plates. To keep bubbles apart requires that a disjoining force is applied (cf. Kähärä et al., Phys. Rev. E, 90 032307, 2014) to nearby interfaces. A force balance applied to each point of a discretised bubble interface then allows the evolution of the foam to be explored.

The talk will illustrate how the method can be used to investigate the flow of foams in porous media, for example, where flow through constrictions and past obstacles provides a method of in-situ foam generation. Experiments in microfluidic channels provide data to validate the method.

Grassia, Paul (University of Strathclyde)
Motion of an oil droplet through a capillary with charged surfaces

A model proposed by Wilmott and co-workers (J. Fluid Mech., vol. 841, pp. 310--350, 2018) for the advance of a charged oil droplet along a charged capillary pore is considered. The oil droplet is surrounded by aqueous phase filling the pore, and the model considers a uniformly curved capillary static droplet front plus a thin aqueous film separating the body of the oil droplet from clay on the capillary wall, with these two regions being joined by a transition region. The methodology follows a classical asymptotic approach proposed by Bretherton (J. Fluid Mech., vol. 10, pp. 166--188, 1961) but incorporates additional electro-osmotic effects (specifically an electro-osmotic disjoining tension) due to the charged surfaces. A number of dimensionless parameters control the model's behaviour of which the most important is denoted χ' and represents the ratio between the "nominal" thickness of the aqueous film (as determined neglecting any electrostatic effects) and the Debye length within the film, which is sensitive to ion concentrations and hence to salinity. When χ' is large, electro-osmotic effects are screened and Bretherton's classical results are recovered. However as χ' decreases, electro-osmotic effects come into play and the film becomes much thicker than Bretherton's prediction so as to ensure that screening effects are not altogether lost, and in addition there is a noticeable increase in the pressure needed to drive the droplet along. These results apply with minor variations in the case of singly charged surfaces (charge on either oil or clay), oil and clay surfaces with like charges, or oil and clay surfaces with opposite but unequal charges. However in the case of opposite and equal charges the system's behaviour changes dramatically. There is now a conjoining electro-osmotic pressure rather than a disjoining tension, the film then becomes thinner than the analogous Bretherton film, and the pressure needed to drive it along decreases. Surprisingly in this case, for sufficiently small χ', the work done by the conjoining pressure can exceed the work done against viscous dissipation, meaning the pressure required to drive the droplet along turns out not just to be smaller than Bretherton's predictions but also to be slightly less than would be estimated based on capillary forces alone.

Hewitt, Duncan (University of Cambridge)
Mud swimming: viscoplastic locomotion and slender-body theory

In the natural environment, a variety of organisms negotiate their way through or across complex fluids, ranging from bacteria and sperm cells immersed in mucus to mudskippers negotiating tidal flats or snails and slugs sliding over their mucus trails. In this talk, a series of basic models of locomotion through viscoplastic fluids - that is, fluids that only deform and flow is the applied stress exceeds some critical yield value - are considered, ranging from Taylor’s two-dimensional swimming sheet to the motion of a helical swimmer. In so doing, a general theoretical framework for viscoplastic slender-body theory is developed and explored. The nonlinearity in the constitutive law for these fluids presents a number of intriguing complications, but also aids the application of slender-body theory, since the stress exerted by an object can only ever deform a localised region of fluid around its body.

With the aid of detailed numerical simulations and asymptotic analysis, a swimming sheet with either transverse and longitudinal waves driving motion is discussed; the flow structures associated with locomotion are explored and an optimum swimming speed is revealed. More generally, a viscoplastic slender-body theory is presented by building on solutions for flow around a cylinder moving either along or perpendicular to its axis. The results are used to the describe sedimentation of cylinders and helices, and, ultimately, to describe mechanisms for helical locomotion through a viscoplastic fluid.

Jiang, Yujie (University of Edinburgh)
Shear-tunability in gel/particle composites

We explore the rheology and structure of binary composites consisting of non-Brownian repulsive particles embedded in a colloidal gel of smaller, attractive particles. Unlike most thixotropic gels, the rheology of composites depends on the flow history in a different way. Rheo-confocal microscopy reveals that vigorous shears lead to a stronger network (gelled state) after shear cessation, whereas moderate shears collapse the attractive gels into disjoint globules (phase-separated state), dramatically increasing the modulus. The reversible transition between the two states offers our composites unique shear-tunability.

King, Jack (University of Manchester)
The Kaye effect: new insights from experiment, theory and modelling
Jack King & Steven Lind (University of Manchester)

The Kaye effect is a phenomenon whereby a jet of fluid poured onto a surface appears to leap on impact, rather than stagnate or coil as expected. Since it was first described in 1963, several authors have attempted to explain the mechanism by which the phenomenon occurs, although to date no complete explanation for the behaviour exists. Current evidence points towards the existence of an air layer between the jet and the heap which enables slip. We show experimentally that the Kaye effect does not occur in a vacuum, indicating that the air layer is crucial for the effect to occur. By conducting a theoretical analysis based on control volumes we show that viscoelasticity plays a key role in the Kaye effect, and this role is two-fold. Firstly, viscoelasticity appears to increase air entrainment, and secondly, it reduces the pressure required to bend the jet, allowing a thicker air layer to be sustained. We present the numerical simulations of viscoelastic jets showing how viscoelasticity qualitatively affects jet buckling, increasing the chances of slip, and therefore the initiation the Kaye effect. These new findings provide insight into a problem that has puzzled rheologists for over half a century.

Lindner, Anke (PMMH-ESPCI)
Dynamics of fibres in viscous fluids

In this presentation we present the individual dynamics of flexible and Brownian filaments under shear and compression. We use actin filaments as a model system and observe their dynamics in microfluidic flow geometries using fluorescent labelling techniques and microscopic tracking methods.

Under shear we characterize successive transitions from tumbling to buckling and finally snake turns as a function of an elasto-viscous number. Under compression we reveal the formation of three dimensional helicoidal structures and characterize their formation.

Finally we attempt at linking the microscopic observations to the macroscopic suspension properties with preliminary measurements of the shear viscosity of dilute suspensions of actin filaments in microfluidic rheometers.

Liverpool, Tanniemola (University of Bristol)
From propulsion mechanisms to collective behaviour of synthetic microswimmers

I will present recent work studying the mechanisms of propulsion and the role of hydrodynamic interactions in the collective behaviour of collections of microscopic man-made catalytic active particles suspended in a fluid. I'll introduce a calculational framework that allows one to separate the different contributions to their collective dynamics from hydrodynamic interactions on different length scales. Hence one is able to quantify the effect of lubrication forces when the particles are very close to each other. I will show that they play as important a role as long-range hydrodynamic interactions in determining their many-body behaviour.

McIlroy, Claire (University of Nottingham)
Modelling amorphous and semi-crystalline polymers in 3D printing
Claire McIlroy & Richard Graham (University of Nottingham), Peter Olmsted (Georgetown University)

The most common method for printing plastics (polymer melts) is known as fused filament fabrication (FFF). This process involves melting a thermoplastic, followed by layer-by-layer extrusion, cooling and re-solidification. The main concern with FFF is the strength at the welds between printed layers; bulk strength is never achieved in these regions and the reason is currently unclear.
We use a molecularly-aware non-isothermal model of the polymer melt to predict how high-shear rates during the deposition process can stretch and align polymer molecules with the flow direction. For amorphous melts, we attribute reduced weld strength to a partially disentangled structure at the onset of the glass transition. For semi-crystalline melts, we explore how the stretch induced by the printing flow can enhance nucleation and lead to a gradient in the number of nuclei across a printed layer.

Papadopoulou, Anastasia (University College London)
Shear rheology and microstructure of particle suspensions in complex oral formulations

Particle suspensions are encountered in a range of healthcare and industrial formulations as well as biological systems. The rheology of particle suspensions is complex and shows non-Newtonian – often unpredictable – flow properties, such as yield stress, shear thinning and shear thickening, even in the case of rigid spheres suspended in Newtonian media. These different phenomena depend significantly on suspension characteristics and the type of deformation applied, and have been widely attributed to particle–particle interactions and changes in the microstructure. In this work, non-aqueous, particle suspensions encountered in oral healthcare formulations are examined.

Steady state and oscillatory shear experiments of smooth glass spheres and rough non-spherical silica particles suspended in glycerol were conducted. Particle surface morphology and roughness were found to increase suspension viscosity and yield stress values and induce non-Newtonian behaviour at lower particle volume fractions. Large amplitude oscillatory shear measurements revealed the rich microstructure changes of the suspensions under shear that lead to non-Newtonian rheology. Additional experiments with mineral oil as the suspending medium were conducted to understand the role of interparticle forces/microstructure on the observed rheological phenomena. Optical shearing techniques are currently in progress to provide a better insight to the microstructure changes occurring under shearing conditions. The work forms part of a research programme on addressing manufacturing challenges of non-aqueous paste formulations.

Poon, Wilson (University of Edinburgh)
Shearing bacterial suspensions

Abstract to follow

Ridley, Tom (University of Leeds)
Computer simulations of packed soft colloids

'Soft' colloids are typically micron or sub-micron scale structured objects such as polymer microgels, which consist of chemically cross-linked polymer networks that are compressible and deformable. Packed soft colloids show rich and complex rheological and flow behaviour and experiments suggest that at packing ratios where the structural dynamics of hard colloids are arrested, a soft colloid system may still be able to undergo cage-breaking due to particle deformation. However, the link between the detailed elastic properties of soft colloids and the resulting dynamics are presently not well understood.

Our simulations utilise a recently developed computational algorithm, Fluctuating Finite Element Analysis, for simulating viscoelastic objects undergoing thermal excitation. While colloidal systems characterised by hard or radially symmetric soft potentials have been much studied, our approach captures the detailed shape deformations of the colloidal particles and ensures that the effect of anisotropic deformation are taken into account. We present results showing the effects of varying effective volume fraction and we find evidence of cage-breaking events continuing to take place even where the effective volume fraction exceeds the volume fraction at which hard colloids become arrested. In addition, we present results of varying material properties and shear rates for a constant effective volume fraction.

Royer, John (University of Edinburgh)
Liquid migration in shear thickening suspensions flowing through constrictions
Rory E O'Neill, John R Royer (presenting author) and Wilson C K Poon

Dense particulate suspensions often become more dilute as they move downstream through a constriction. We find that as a shear-thickening suspension is extruded through a narrow die and undergoes such liquid migration, the extrudate maintains a steady concentration ϕ_c, independent of time or initial concentration. This concentration ϕ_c varies with volumetric flow rate Q and die radius $r_{\rm d}$, but at low Q collapses onto a universal function of $Q/r_{\rm d}^3$, a characteristic shear rate in the die. We explain quantitatively the onset of liquid migration in extrusion by coupling a recent model for discontinuous shear thickening and the `suspension balance model' for solvent permeation through particles.

Singh, Shiwani (University of Warwick)
A new class of multiscale models for polymeric fluid dynamics

Despite its ubiquity and importance, most of our predictive knowledge of polymer-flow interactions comes from computational modeling based on ad-hoc closure approximations which are well known to fail in regions of high strain. We propose a computationally efficient multi-scale modeling approach for polymer solutions wherein the polymer-solvent coupling occurs in velocity phase space using a Boltzmann-type collision dynamics; rendering the closure approximations unnecessary. The collision between the polymer dumbbell and solvent molecule is modeled using a quasi-equilibrium based relaxation collision kernel and discrete numerical scheme is inspired by the lattice Boltzmann method. Via numerical simulations of Kolmogorov flow, we show that the proposed solvent-polymer coupling strategy successfully captures the following two opposite effect exhibited by polymer solutions: (a) the substantial reduction of the drag in turbulent flow limit and (b) the trigger of chaotic flow in the inertia-free limit, arising solely due to interaction of the elasticity of polymer with the flow, also known as ‘elastic-turbulence’.

Stewart,Peter (University of Glasgow)
Fracture dynamics in foam: Finite-size effects
Peter Stewart and Sascha Hilgenfeldt, University of Illinois Urbana Champaign

Injection of a gas into a gas/liquid foam is known to give rise to instability phenomena on a variety of time and length scales. Macroscopically, one observes a propagating gas-filled structure that can display properties of liquid finger propagation as well as of fracture in solids. Using a discrete model, which incorporates the underlying film instability as well as viscous resistance from the moving liquid structures, we describe brittle cleavage phenomena in line with experimental observations. We find that the dimensions of the foam sample significantly affect the speed of the cracks as well as the pressure necessary to sustain them: cracks in wider samples travel faster at a given driving stress, but are able to avoid arrest and maintain propagation at a lower pressure (the velocity gap becomes smaller). The system thus becomes a study case for stress concentration and the transition between discrete and continuum systems in dynamical fracture; taking into account the finite dimensions of the system improves agreement with experiment.

Townsend, Adam (Imperial College London)
Simulating flexible filament suspensions and their sedimentation

Microscopic flexible filaments and rigid fibres suspended in and interacting with fluids arise in many industrial processes and biological contexts and, due to their elasticity, are a staple ingredient of non-Newtonian fluids. In this talk, we present a comprehensive, scalable methodology for simulating suspensions of flexible filaments, overcoming time-step limitations due to numerical stiffness while also resolving fully 3D filament deformations due to bending and twisting through the use of quaternions. Using this approach, we examine the dynamics of sedimenting filaments in isolation, in small groups, and, finally, in large clouds and in homogeneous suspensions, and compare our results with those found previously for rigid filaments. Our simulations show how flexibility can complicate, but also simplify filament trajectories, and lead to enhanced settling speeds and non-trivial dynamics in large clouds.

Wilson, Stephen (University of Strathclyde)
Rivulet flow of Generalised Newtonian Fluids
This is joint work with Dr F H H Al Mukahal (King Faisal University) and Dr B R Duffy (University of Strathclyde)

Steady unidirectional gravity-driven flow of a uniform thin rivulet (ie a rivulet with small transverse aspect ratio) of a generalised Newtonian fluid down a vertical planar substrate is considered. The parametric solution for any generalised Newtonian fluid whose viscosity can be expressed as a function of the shear rate, and the explicit solution for any generalised Newtonian fluid whose viscosity can be expressed as a function of the extra stress are obtained. These general solutions are used to describe rivulet flow of Carreau and Ellis fluids, highlighting the similarities and differences between the behaviour of these two fluids.
(This is joint work with Dr F H H Al Mukahal (King Faisal University) and Dr B. R. Duffy (University of Strathclyde)).

Al Mukahal, F.H.H., Duffy, B.R., Wilson, S.K., Rivulet flow of generalized Newtonian fluids, Phys. Rev. Fluids 3, 083302 (2018)