IChemE
Fluid Mixing Processes
Special Interest Group

Multiphase flow and mixing dynamics for the chemical and biopharma industries

Friday 16th September 2022, Hybrid Mode (*Please register at this link*)

Physical Venue: Design Suite, Level 4 Bernard Katz Building, Main UCL Campus[1] (*Link*)

Arrivals		
10:30-11:00	Welcome and refreshment	
Event Introduction		
11:00 – 11:10	Welcome and introduction to the day	**Andrea Ducci**
Chair: Andrea Ducci and Martina Micheletti		
11:10 – 11:30	Investigating the effects of process variables on torque measurements to improve the scale-up of structured liquids	**Grace E. Cunningham,** School of Chemical Engineering, University of Birmingham, Unilever Research and Development
11:30 – 11:50	Resolvent analysis of turbulent pipe flow laden with low-inertia particles	**Rasmus Korslund Schlander,** Department of Aeronautics, Imperial College London
11:50 – 12:10	Mixing, Power number and flow dynamics of a scale-down prototype of the single-use Allegro™ STR bioreactor	**Jordan Delbridge,** Biochemical Engineering, UCL
12:10 – 13:30	**Lunch/Coffee Break**	
13:30 – 13:50	Modelling of pipe flow to understand mixing in the transitional flow regime	**Georgina Wadsley,** School of Chemical Engineering, University of Birmingham
13:50 – 14:10	Viscoelasticity-induced particle migration in stirred vessels	**Giovanni Meridiano,** Chemical Engineering Department, UCL
14:10 – 14:30	Imaging and ultrasound techniques for dispersed drop size measurements in stirred vessels	**Xueyu Qi,** Chemical Engineering Department, UCL
14:30 – 15:00	Wrap-up and prizes announcement	**Richard Fyles,** FMG Chair
15:00 Close		

[1] Get in touch with the event organiser, Dr Andrea Ducci (a.ducci@ucl.ac.uk), for directions and any other matter.

List of Abstracts

Investigating the effects of process variables on torque measurements to improve the scale-up of structured liquids

Grace E. Cunningham[1,2], Shreyasi Deshpande[1], Mark J.H. Simmons[1], Jonathan J. O'Sullivan[2]

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ABSTRACT
The manufacture of formulated products such as structured liquids is typically achieved through batch processing, where materials are added to the process vessel sequentially. As the product microstructure is dependent on both the formulation (ingredients and their associated inclusion levels) and the processing steps employed, process conditions such as order and rate of addition, temperature profiles and mixing profiles are carefully designed and controlled with the aim of ensuring the optimal product structure is formed. The rheology of the contents evolve as the batch progresses, relative to the incipient product microstructure. In order to optimise both process and product, it would be beneficial to understand more about how the rheology is evolving and affected by process conditions.
A relatively simple and cost-effective process monitoring technique is the measurement of torque required to turn the agitator shaft. In the laminar mixing regime, torque can be related to viscosity using a variety of techniques, developed over the years by researchers investigating different types of agitators and fluid rheology, *e.g.,* Matching Viscosity Method (MVM) [1] [2], Torque Curve Method (TCM) [3] and the Couette analogy [4] [5]. However, none of these approaches have considered if it is possible to infer viscosity from torque measurements when the batch fill level is less than 100% *i.e.,* before the addition of all of the raw materials. The aim of this work is to determine if any of these methods (MVM, TCM and Couette analogy) are suitable for measuring viscosity from torque at less than 100% batch fill levels for close clearance agitator systems such as helical ribbons and agitators. Torque measurements have been taken at three different fill levels (25%, 62.5%, 100%) at a range of speeds (0.125 m/s – 1.5 m/s) for three different geometries (Figure 1) and four types of rheology fluids (Table 1), using a DHR rheometer (TA Instruments, UK). The mixer viscometry techniques mentioned above were applied to each fill level, fluid and geometry to determine the suitability of the method for each situation.

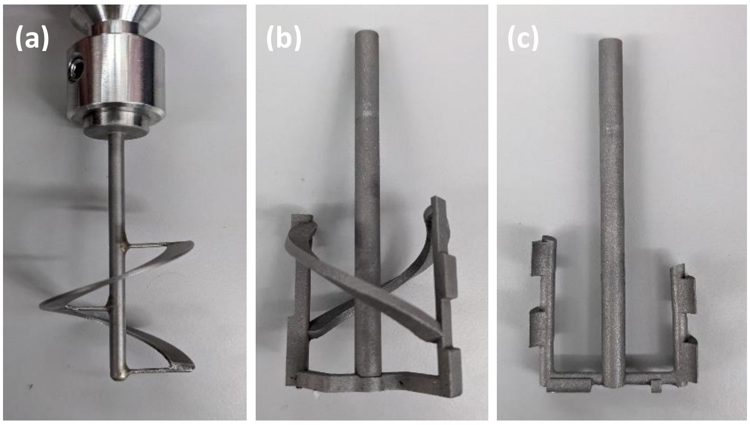

Figure 1 – (a) TA Instruments helical rotor (TA-HR), (b) 3D printed helical ribbon (3D-HR), and (c) 3D printed anchor (3D-ANC)

Table 1 - Consistency index and flow index of the fluids investigated

Fluid	**Consistency index, K, Pa.s^n (or viscosity for Newtonian fluid)**	**Flow index, n, -**
Glycerol	0.56	-
Model conditioner	186	0.06
Xanthan gum	70	0.16
1.5% Carbopol	99	0.20

Results showed that for extremely shear-thinning fluids like the model hair conditioner, the Couette analogy is not suitable. The MVM and TCM approaches also failed to accurately predict viscosities and shear rates at low fill levels due to reduced torque responses. In light of the lack of suitability of current methods, an artificial neural network (ANN) was applied to the data to investigate the appropriateness. Initial results showed that apparent viscosity could be estimated using fill level, RPM, geometry mass and torque as inputs (R^2 = 0.85, RMSE = 0.731), which serves as a promising basis for a process monitoring and optimisation tool.

References

[1] A. Metzner and R. Otto, "Agitation of non-Newtonian fluids," *AIChE Journal,* vol. 3, no. 1, 1957.

[2] K. Mackey, R. Morgan and J. Steffe, "Effects of shear-thinning behaviour on mixer viscometry techniques," *Journal of Texture Studies,* vol. 18, pp. 231-240, 1987.

[3] M. E. Castell-Perez and J. F. Steffe, "Evaluating shear rates for power law fluids in mixer viscometry," *Journal of Texture Studies,* vol. 21, pp. 439-453, 1990.

[4] L. Choplin and P. Marchal, "Mixer-Type Rheometry," in *Rheology*, vol. 2, EOLSS Publications, 2010.

[5] A. Ait-Kadi, P. Marchal, L. Choplin, A.-S. Chrissemant and M. Bousmina, "Quantitative Analysis of Mixer-Type Rheometers using the Couette Analogy," *The Canadian Journal of Chemical Engineering,* vol. 80, 2002.

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Resolvent analysis of turbulent pipe flow laden with low-inertia particles

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ABSTRACT

We extend the resolvent framework to turbulent flows laden with low-inertia particles. The particle velocities are modelled using the equilibrium Eulerian model, which is valid for Stokes numbers up to 1. We analyse a vertical turbulent pipe flow with a Reynolds number of 5300 based on diameter and bulk velocity, for Froude numbers Fr_z=-4,-0.4,0.4,4 as well as the special case $1/Fr_z=0$ where gravity is omitted and Stokes numbers St^+=0-1. A direct numerical simulation (DNS) for a pipe with a length of 7.5 diameters (*D*) is performed with the particles released uniformly at the pipe inlet. The particles are re-inserted from the outlet to the inlet in order to artificially increase the domain length and it is shown that the mean concentration profiles become self-similar around 12*D* downstream of the inlet. The concentration profiles from the DNS are then used in the resolvent framework. The resolvent formulation can predict some of the physical phenomena observed in inertial particle flows such as localized high concentration due to the vortical centrifuge effect, turbophoresis and gravitational effects. It also reveals that the upward flow increases particle concentration in the log layer of the pipe and that the downward flow increases concentration near the centre of the pipe. Both phenomena have been observed in previous Lagrangian simulations as well as experiments. The main effect of increasing the Stokes number is the amplification of smaller streamwise wavelengths which indicates an increase of local scale clustering of particles. It was also found that increasing the Stokes number increases turbophoresis. The effect of the direction of gravity was also reproduced using a simplified resolvent model, which did not require a mean concentration profile as input. This Resolvent model simplifies the analysis since no prior simulation or experiment is required for the model to work. Finally, the particle wall deposition rate is analysed, and it is observed that the azimuthal modes k_θ=3-6 have a larger impact on deposition compared to other azimuthal modes and that these modes seem to be suppressed with increasing Stokes number for an upward flow.

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Mixing, Power number and flow dynamics of a scale-down prototype of the single-use Allegro™ STR bioreactor

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ABSTRACT

Optimisation of cell culture conditions in industry scale stirred tank reactors (STRs) is crucial to the successful development of new biopharmaceuticals with commercially feasible quality and yields. The growing use of single-use bioreactors has facilitated in reducing process costs significantly. While the traditional dished head cylindrical tank has been the tried and tested method of large-scale cell culture for decades, novel commercial STRS are being adapted for improved practicality and based on years of research in the field of mixing. The Allegro STR range is one such design, which was used in the rapid development and production of the ChAdOx1 nCoV-19 vaccine, where low costs and high productivity were achieved with consistent product quality across the scale [1]. This novel bioreactor design has a cubical biocontainer, three large asymmetrically placed wedge-shaped baffles, and a low shear elephant ear (EE) impeller. To explore the implications of this unique geometry on power consumption, mixing, and flow dynamics, a 1 L transparent mimic of the 50-2000 L commercial range was developed and compared to that of an EE impeller in a 'standard' baffled cylindrical configuration of equivalent geometric proportions. The large baffles and square cross section of the Allegro STR saw an increased power consumption, reduced mixing times, and an asymmetric flow structure compared to that in the standard STR.

References

[1] Joe, C. C. D. *et al.* Manufacturing a chimpanzee adenovirus-vectored SARS-CoV-2 vaccine to meet global needs. *Biotechnol. Bioeng.* **119**, 48–58 (2022).

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Modelling of pipe flow to understand mixing in the transitional flow regime

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ABSTRACT

Validated Computational Fluid Dynamics (CFD) simulations when applied to industrial flows are powerful predictive tools that facilitate rapid modification of existing batch mixing processes to increase efficiency, reduce energy consumption, and aid with scale-up and scale-down approaches. Over the last two decades, numerous experimental and numerical studies have explored the hydrodynamics of liquid flows in stirred tanks and pipes for a wide range of fully turbulent and laminar cases that are now applied in manufacturing industries [1]. However, many home, personal care, and food products develop a complex functional microstructure, due to the inclusion of high concentrations of thickeners and surfactants. This causes an evolution of their rheology during manufacture. It is therefore possible for industrial fluids to vary from low to high apparent viscosity during processing as the microstructure builds, transitioning from the turbulent, through transitional, to the laminar flow regime. In the transitional flow regime, where current research is limited, hydrodynamic instabilities create unsteady flows that are difficult to predict [2].

The current study aims to advance the understanding of transitional flow and its characteristics in a pipe with a constant perturbation provided by a square edged orifice plate, encouraging transition to turbulence. During the initial stages of testing CFD closure models, pipe flows were selected to provide the benefit of a simpler geometry and more predictable local flow behaviour than stirred tanks. Particle Image Velocimetry (PIV) measurements are used to identify flow phenomena and provide experimental data to validate the application of CFD turbulence closure models (generalised k-ω (GEKO) and stress blended eddy simulation (SBES)), as well as a laminar model, using ANSYS Fluent (version 2021R2) software.

Following a mesh independence study with water, a polyhexcore mesh of ~ 350k cells was selected for subsequent simulations. Unsteady flows of two Newtonian fluids 50 wt% glycerol ($\mu = 0.00555$ Pa s) and 60 wt% glycerol ($\mu = 0.00940$ Pa s) where measured using PIV at a range of flow rates corresponding to known Reynolds number flows (Re 300 – 6,000), selected to cover the transitional regime and identify laminar and turbulent limits. PIV and CFD data are compared to determine which closure model (laminar, GEKO or SBES) most accurately predicts the hydrodynamics of transitional flow, thus determining suitability or potential modifications. The boundaries at which the system evolves between laminar, transitional, and turbulent regimes and, therefore, where to use the most appropriate closure models is also assessed. This research will later return to investigate transitional flow in a stirred tank with a similar investigative approach, applying the knowledge gained from the pipe flow study.

References

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Viscoelasticity-induced particle migration in stirred vessels

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ABSTRACT

In this study, we investigate the viscoelasticity-induced migration of solid particles immerged in the three-dimensional flow field created by the rotation of a Rushton turbine. At the same time, we propose a scaling law for predicting the characteristic particle migration time as a function of the Weissenberg number. Particle image velocimetry is adopted to reconstruct the three-dimensional velocity and deformation rate fields generated by the rotation of the Rushton turbine in both Newtonian and viscoelastic fluids; concurrently, particle tracking is used to measure the evolution of the particle distribution in the tank. The experimental campaign shows that the deformation rate field is essentially bi-dimensional and confined to the *r*-*θ* plane. Accordingly, the particles migrate only in the radial direction driven by the presence of gradients of shear rate on the *r*-*θ* plane. Finally, the scaling law is validated against experimental data obtained at different Weissenberg numbers, impeller diameters and fluid compositions. The results show good agreement between the scaling law and the experimental data.

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Imaging and ultrasound techniques for dispersed drop size measurements in stirred vessels

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ABSTRACT

Two phase dispersed flows of immiscible liquids in stirred vessels are of great importance in industry including chemical, food and pharmaceutical applications. The drop sizes depend on the two opposing phenomena of drop breakage and coalescence and play a significant role in such a process, as they affect the rheology of the mixtures and the mass transfer rates; the measurement of drop size distributions in dispersed systems will help to understand and predict multiphase flows. From the various measurement methods available, ultrasound techniques are cheap, harmless, easy to setup and can be applied to non-transparent test sections; they can also be used for fast, online measurements in small and large scales systems.

In this work we develop non-intrusive ultrasound diagnostic techniques for the measurement of the drop sizes and their distributions in stirred tanks. For the validation of the ultrasound results, planar laser induced fluorescence (PLIF) technique was used to image the drops at the same time and location as that of the ultrasound transducers. The study was carried out in a small-scale stirred vessel made of acrylic pipe with ID of 50 mm, that was enclosed in a square box (See Fig. 1). The test fluids were silicone oil (density 915 kg m^{-3} and sound speed 1014 m/s) and a water/glycerol mixture (density 1124 kg m^{-3} and sound speed 1670 m/s). The two liquid phases had matching refractive index to enable imaging. The ultrasound techniques applied here are based on the measurement of the attenuation coefficient for particle sizing, and on the sound speed for the volume fraction analysis. For the PLIF studies, a high frame rate Photron camera and a continuous Diode-Pumped Solid-State (DPSS) laser were used to provide high resolution information of the drop size distribution at a longitudinal section of the vessel. The experimental setup, methodology and data post-processing for obtaining droplet volume fraction and size distributions will be discussed.

The ultrasound propagation speed for the silicone oil dispersion in water/glycerol was found to be between 1601 m/s and 1662 m/s for droplet volume fractions spanning from 0.53% to 4.2%. The droplet size distributions, measured by both ultrasound and PLIF, ranged from 0.25 mm to 2 mm, and were in very good agreement between the two techniques (see Fig. 2). The results indicated that ultrasound technique is a powerful tool for characterizing dispersed phases in liquid-liquid dispersed flows.

(a) (b)

Figure 2: Experimental setup of (a) planar laser induced fluorescence (PLIF) and (b) ultrasound instruments (T1-transmitting transducer, T2-receiving transducer).

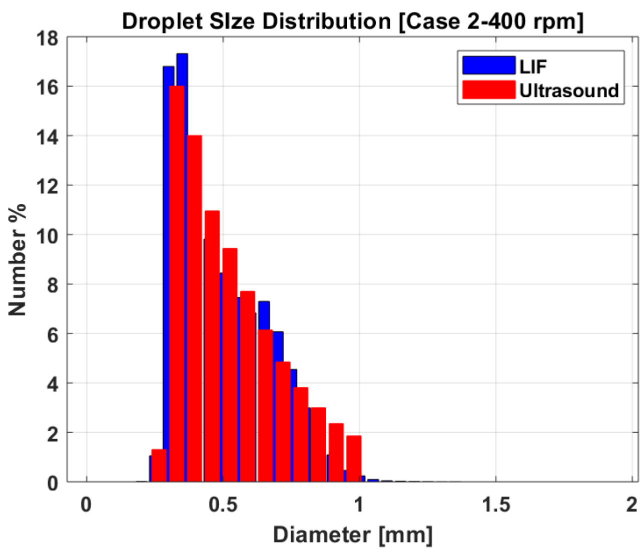

Figure 2: Droplet size distribution from the measured attenuation coefficient of silicone oil droplets in water/glycerol continuous phase [red bars] and from laser induced fluorescence [blue bars], when impeller is located approximately 25 mm below the interface and rotates at 400 rpm with 0.1 oil volume fraction.

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