UK Fluids Network

Special Interest Group 10

Fluid Mechanics of Cleaning and Decontamination

Summer 2018 Conference

29th-30th August 2018

Isaac Newton Institute

Clarkson Road

Cambridge CB3 0EH

Programme

Wednesday 29th August

9:00	Registration
9:30	Conference Opening
9:45	***Plenary Lecture A*** Movement of contaminants through cities and buildings *Prof. Paul Linden, University of Cambridge*
10:40	**MORNING BREAK**
11:00	Heat transfer in locally-heated falling liquid films *Dr Alice Thompson, University of Manchester*
11:20	A combined experimental and theoretical study of cleaning in the pharmaceutical industry *Dr Vincent Cregan, University of Limerick*
11:40	Liquid sprays used in batch cleaning *Alistair Rodgers, University of Leeds*
12:00	Applications of water jetting in the nuclear industry *Gareth Yates, Sellafield Ltd*
12:20	Laminar to turbulent transition in the flow field created by impinging liquid jets; effect on cleaning and heat transfer *Rajesh Kumar Bhagat, University of Cambridge*
12:40	Recent results on the cleaning of a starch layer by a liquid jet and its prediction *Matthias Joppa, Technische Universität Dresden*
13:00	**LUNCH**
14:00	***Plenary Lecture B*** The use of bubble acoustics in cleaning and decontamination *Prof. Timothy Leighton, University of Southampton*
15:00	Bubble propagation in Hele-Shaw channels with centred constrictions *Prof. Anne Juel, University of Manchester*
15:20 *P*	Cleaning patterns on curved walls *Melissa Chee, University of Cambridge*
15:25 *P*	Spreading of contaminant in the intermediate stages of decontamination *Daniil Slavin, University of Cambridge*
15:30 *P*	Monitoring the release of mobile oils from burnt food mixtures *Nathan Ravoisin, University of Cambridge*
15:35 *P*	Modelling of erosion of thin deposited soils by impinging liquid jets *Prof. Ian Wilson, University of Cambridge*
15:40 *P*	Modelling of coupled deformation of viscoplastic layers and fluid dynamic gauging flows using two-phase CFD *Jheng-Han Tsai, University of Cambridge*
15:45	**EXTENDED TEA BREAK AND POSTER SESSION**

Programme

Wednesday 29th August

16:20	The development and initial testing of the ice pig cleaning method for nuclear reprocessing plants *Alex Jenkins, Sellafield Ltd*
16:40	Experimental study of displacement of a Newtonian fluid by shear-thinning solutions *Evangelina Roumpea, University College London*
17:00	Three-dimensional DNS of product changeover *Dr Lyes Kahouadji, Imperial College London*
17:20	Using electrical resistance tomography (ERT) to monitor the removal of a non-Newtonian soil by water from a cleaning-in-place (CIP) circuit containing different pipe geometries *Dr Peter Martin, University of Manchester*
17:40	Use of machine learning algorithms for prediction of cleaning efficiency of product changeover process *Dr Aditya Karnik, Imperial College London*
18:00	**SUMMARY OF DAY**
19:30	**DRINKS RECEPTION AND CONFERENCE DINNER** Main Hall, Jesus College

Jesus College
Jesus Lane
Cambridge
CB5 8BL

Programme

Thursday 30th August

9:00	***Plenary Lecture C*** What a fluid mechanistic needs to know about surfactants *Prof. Stuart Clarke, University of Cambridge*
10:00	Methods of monitoring cleaning in situ *Georgina Cuckston, University of Cambridge*
10:20	Experimental study of the removal of bulk contaminant droplets using an ionic liquid simulant *Dr Merlin Etzold, University of Cambridge*
10:40	Drop dynamics on liquid infused surfaces *Dr Halim Kusumaatmaja, Durham University*
11:00	**MORNING BREAK**
11:20	Experimental derivation of chemical evaporation rates from unclothed and clothed sebum-coated discs under various exposure conditions *Dr Hazem Matar, University of Hertfordshire*
11:40	The influence of the thermal properties of the system on the lifetime of an evaporating droplet *Feargus Schofield, University of Strathclyde*
12:00	Numerical simulations of moving contact lines *Dr Yi Sui, Queen Mary University of London*
12:20	Surface permeability and capillary transport *Dr Alex Lukiyanov, University of Reading*
12:40	Gas nanofilms in drop impact and spreading *Dr James Sprittles, University of Warwick*
13:00	**LUNCH**
14:00	Homogenisation of agents and cleansers interacting on a microscale *Ellen Luckins, University of Oxford*
14:20	Decontamination in cracks and fractures *Dr Julien Landel, University of Manchester*
14:40	Modelling unsaturated decontamination *Oliver Whitehead, Univesity of Oxford*
15:00	Impinging water jet cleaning of a hydrophobic non-Newtonian soil on flat surfaces *Rubens Rosario Fernandes, University of Cambridge*
15:20	**CONFERENCE CLOSE**
15:45	**TOUR OF GK BATCHELOR LABORATORY**

9:45 ***Plenary Lecture A***

Movement of contaminants through cities and buildings

Paul Linden

Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK

The imperative to reduce energy consumption in cities drives a need to replace air conditioning with other forms of low-energy ventilation in buildings. Natural ventilation is an obvious candidate and, since it requires exchange between the interior of a building and the outside environment, the relative level of a contaminant inside and outside is very important in determining the quality of the internal environment.

In this talk I will describe the basic fluid mechanics behind low-energy natural ventilation and the implications for contaminant movement within buildings. I will show that depending on the location of the pollution source the distribution within a building can differ significantly from one case to another. Using results from a recent field study in London I will also show that pollution levels in the city vary significantly in time and space and that these variations must be taken into account when operating a naturally ventilated building. Finally, I will discuss an ongoing project that aims to provide an integrated modelling system that will provide a tool to make accurate assessments of the potential to reduce energy consumption and excess heat emissions from buildings.

MORNING BREAK

11:00 Heat transfer in locally-heated falling liquid films

Alice Thompson*, Susana Gomes, Michael Dallaston, Fabian Denner and Serafim Kalliadasis*

School of Mathematics, University of Manchester, UK

Imperial College, London, UK

University of Coventry, UK

Falling liquid films can be passively or actively controlled by the application of spatially and temporally non-uniform inputs such as substrate heating, mass injection or moving topography. We focus here on substrate heating, and assume that the imposed heating affects the film dynamics only through temperature-dependent surface tension.

The question of how the substrate temperature affects the surface temperature is non-trivial, and in fact existing modelling methodologies either fail to respect fundamental thermodynamic properties or else do not accurately capture the effects of advection and diffusion on the temperature profile. We argue that the best performing long-wave models are those that give the surface temperature implicitly as the solution of an evolution equation in which the wall temperature (and none of its derivatives) appears as a source term. We test this model in linear and nonlinear regimes at moderate Reynolds number, and show that its predictions are in remarkablly good quantitative agreement regarding the surface temperature, the internal temperature field, and the interface displacement that would result from temperature-induced Marangoni stresses. Finally, we discuss how the modelling methodology can be extended to other thin-film systems including cleaning and decontamination problems.

11:20 A combined experimental and theoretical study of cleaning in the pharmaceutical industry

***Vincent Cregan**, Cameron Hall and Darren Whitakter*
PMTC/MACSI, University of Limerick, Ireland

Cleaning in the pharmaceutical industry is time consuming and costly. To prevent drug product cross contamination, cleaning occurs during product changeovers. Recently, the frequency of cleaning has increased dramatically due to the increased focus on smaller production volumes and shorter campaigns. The resulting increase in product changeovers has led to more cleaning. Consequently, there is a demand for optimal strategies that minimise the time and resources spent on cleaning.

To simulate cleaning in the pharmaceutical manufacturing industry, the PMTC constructed a small-scale cleaning rig to simulate a liquid flowing over an active pharmaceutical ingredient (API) on an inclined surface. As the liquid washes over the API and runs off, a UV-VIS spectrophotometer is used to measure the API concentration in the liquid as a function of time.

The experimental data is modelled via a system of differential equations composed of the equations of motion of the liquid and an advection-diffusion equation for the residue concentration in the liquid. Dimensional analysis is used to display the relative importance of advection and diffusion with respect to API removal. The solutions to the model are used to ascertain the key physical factors which affect cleaning.

Acknowledgements: The authors are grateful for the financial support of the Pharmaceutical Manufacturing Technology Centre (an Enterprise Ireland & IDA Initiative) and the Mathematics Applications Consortium for Science and Industry (funded by Science Foundation Ireland grant no. 12/IA/1683).

11:40 Liquid sprays used in batch cleaning

***Alistair Rodgers**, Nik Kapur, Gregory De Boer and Gordon Scott*
Department of Mechanical Engineering, University of Leeds, UK
GSK, UK

The purpose of this research is to further the understanding of cleaning processes observed in the manufacturing of pharmaceutical products by investigating the mechanisms of liquid sprays impinging on soiled surfaces. In practice there are a small number of components that do not satisfy the established cleanliness criteria after being cleaned, this is a source of inefficiency to which this research will seek to characterise and minimise. Recent articles have explored the fundamentals of cleaning due to fluids impinging on soiled surfaces, however the underlying mechanisms of soil removal via sprays remain unexplored.

Experimental work was carried out on a test rig to simulate the cleaning of components in cleaning processes carried out within the pharmaceutical industry. A spray was set up to impinge against a vertical Perspex wall coated with white soft paraffin, an excipient commonly used in pharmaceuticals processing. Tests were run using water across a range of temperature with no surfactant and recorded using a video camera in order to observe the cleaning process. A novel feature of this research is a direct comparison between the basic mechanisms of soil removal due to sprays, as opposed to the more frequently studied jet. Cleaning performance was measured as a function of the volume of paraffin removed and the energy required to achieve this.

Supporting computational work was carried out on COMSOL, observing single droplets of water impinging on a liquid film. This allowed the interaction of the droplets with the substrate to be viewed in more detail and subsequently a further understanding of the mechanism by which the spray removes a soil from the surface.

12:00 Applications of water jetting in the nuclear industry

***Gareth Yates**, Alex Jenkins and Liz Ostle*
Sellafield Ltd, Seascale, UK

Water jetting is a decontamination tool with a plethora of applications. Within the nuclear industry, water jetting with and without abrasive media is becoming more widely used for coatings removal, blockage removal, cutting and decontamination. With future decommissioning challenges of the industry moving closer, more widespread use of the technology is anticipated, building upon the examples of use to date. Additional precautions are required to be used in the nuclear industry, which renders some possible options challenging to deliver.

We will illustrate how High Pressure and Ultra High Pressure water jet systems ranging from 200 bar to 3000 bar have been used. It is advantageous to appreciate why a given method was selected noting that work-rate is often not a key consideration. Actual works will be illustrated, discussing the challenges and benefits of deploying 'new' technologies within a traditionally risk adverse industry.

12:20 Laminar to turbulent transition in the flow field created by impinging liquid jets; effect on cleaning and heat transfer

***Rajesh Kumar Bhagat** and Ian Wilson*
Department of Chemical Engineering and Biotechnology, University of Cambridge, UK

Impinging liquid jets are widely used for cleaning (such as cleaning-in-place) and heat transfer applications. Bhagat and Wilson (2016, *Chem. Eng. Sci*, **152**, 606-623) studied the flow field created by turbulent water jets on vertical walls and showed that impinging jets generate four regions of different hydraulic action. At the point where the jet impinges (the stagnation point) hydraulic action is present as vibration, water hammer, and other normal forces associated with transfer of momentum towards the wall, as well as an increase in wall shear stress from r = 0 to the jet radius r_o. In the remainder of the radial flow zone (RFZ, from r_o to the film jump) the liquid flow passes through stages of a boundary layer formation zone; laminar flow; and a turbulent zone. The shear stress exerted on the wall generally decreases with r, but passes through a local maximum at the location of the laminar to turbulent transition. Cleaning of a model food soil such as Xanthan gum, for which the cleaning mechanism involves shear-driven removal and dissolution, features a doughnut-shaped cleaned region in the early stages. A cleaning front develops at the point of impingement and moves radially outwards while, simultaneously, another cleaning front develops as a ring at radial location r_t, in the RFZ. We hypothesise that this second cleaning front develops at a location where the laminar liquid film becomes turbulent. We present measurements of the laminar to turbulent transition and compare the results with cleaning and heat transfer data.

12:40 Recent results on the cleaning of a starch layer by a liquid jet and its prediction

Matthias Joppa, *Hannes Köhler, Jochen Fröhlich, Jens-Peter Majschak and Frank Rüdiger*

Technische Universität Dresden, Institute of Natural Materials Technology, Dresden, Germany

Technische Universität Dresden, Institute of Fluid Mechanics, Dresden, Germany

Industrial cleaning applications for large tanks, *e.g.* in the food and beverage industry, mainly use rotary jet cleaners to remove tenacious soils. Despite this frequent use and lately increasing research interest on that topic, the mechanics of jet cleaning are still not fully revealed. The results are suboptimal cleaning protocols and an increased consumption of resources. In a multidisciplinary approach the present authors combine the measurement of cleaning and flow related quantities with simulations using computational fluid dynamics to examine the cleaning behaviour of impinging liquid jets on the one hand and develop models to predict the cleaning process on the other hand. These efforts resulted in a validated model for the cleaning of swellable soils which are removed by cohesive separation of small particles.

Here, the computational model is applied to predict the cleaning results of a water jet impinging on a dry layer of waxy maize starch for jet Reynolds numbers up to 50 000 and a dimensionless distance between nozzle with diameter D and impingement plate up to L/D = 120. The generation of the model is described with special focus on the fluid mechanical properties of the jet including surface instabilities. Finally, the predicted cleaning times are compared to experimental values. The simulation approach includes a scale up from a parametrization in a bench-scale channel flow to jet cleaning which is associated with a change in wall shear stress of more than one order of magnitude. Nevertheless, the results are in good agreement.

LUNCH

14:00 ***Plenary Lecture B***

The use of bubble acoustics in cleaning and decontamination

Timothy Leighton

Institute of Sound and Vibration Research, Faculty of Engineering and the Environment, University of Southampton, UK

Gas bubbles in liquids couple extraordinarily well to acoustic fields. In response to an oscillating pressure field, bubbles undergo volume changes with a well-defined resonance frequency that depends on the bubble size, the gas providing the compressibility of this nonlinear oscillator, and the liquid providing the inertia. As a result, they generate and scatter sound fields, and can cause physical, chemical and biological changes to material in the vicinity of the bubble. This talk discusses the cleaning and decontamination effects that can be produced when the acoustic field is tuned to generate an instability on the bubble wall as it pulsates, generating surface waves on the bubbles wall, which in turn cause convection in the liquid around it.

15:00 Bubble propagation in Hele-Shaw channels with centred constrictions

***Anne Juel**, A. Franco-Gomez, A.L. Hazel and A.B. Thompson*

School of Physics & Astronomy, University of Manchester, UK

We investigate steady and transient two-phase displacements in a Hele-Shaw channel – a channel of large width to depth ratio – by either injecting air into the oil filled channel or driving a finite bubble with constant flow rate. We demonstrate that a simple change in the bounding geometry of the containing vessel, *e.g.* a small height constriction within the cross-section of a rectangular channel, can radically alter the behavior of a fluid-displacing air bubbles and fingers.

A rich array of propagation modes, including symmetric, asymmetric and localized fingers, is uncovered when air displaces oil from axially uniform tubes that have local variations in flow resistance within their cross-sections. In addition, oscillatory fingers arise when the finger lies on the edge of the height constriction through a mechanism of periodic sideways motion of the interface at a fixed relative distance behind the moving finger-tip. We apply these findings to passively sort bubbles by size.

We support our experimental findings with a complementary analysis based on a depth-averaged theory. The theoretical study reveals that the exchange of stability between different modes of bubble propagation relies on non-trivial interactions between capillary and viscous forces.

15:20 ***P*** Cleaning patterns on curved walls

Melissa Chee *and Ian Wilson*
Department of Chemical Engineering and Biotechnology, University of Cambridge, UK

The effect of wall curvature on the cleaning pattern generated by a horizontal impinging water jet was investigated for coherent jets of 2 mm diameter. The jet Reynolds numbers were in the range of 4000 – 21000. Four Perspex cylinders were used with inner diameter, D, between 10 and 29 cm, and the wall curvatures were in the range of 7 – 20 m^{-1}. The relationship between the half-width of the radial flow zone at the level of the point of impingement, R, and the half-width of the wetted region at the level of the point of impingement, R_c, was found to be R_c = (4/3) R at higher jet Reynolds numbers, and between R_c = (4/3)R and R_c = 2 R at lower jet Reynolds numbers. This is broadly consistent with the work of Wilson *et al*. (2012, *Chem. Eng. Sci*., 68, 449-460) on flat walls, suggesting that wall curvature does not affect the relationship between R and R_c. At lower jet Reynolds numbers, R was found to be insensitive to curvature (within experimental error). At higher jet Reynolds numbers of 19 000 and above, there was a slight decrease in R with increasing curvature. One explanation for the decrease in R could be that splatter mechanisms are affected by wall curvature, as significant splatter is observed on flat walls at these higher jet Reynolds numbers. Larger jet diameters and higher jet Reynolds numbers were also investigated, and 'wraparound' flow patterns were observed.

15:25 ***P*** Spreading of contaminant in the intermediate stages of decontamination

Daniil Slavin*, Merlin Ertzold and Stuart Dalziel*
Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK

Decontamination using surface washing techniques results in the contaminant being spread unless aggressive chemicals capable of almost instant deactivation of the contaminant are used. Spreading the contaminant on an absorbing surface may increase the contaminated area and therefore the associated hazards.

Experimental modelling of such processes is complicated, since simulants and substrates with suitable properties are difficult to find and sometimes source. The most important of these properties is ease of detectability. We explored different dyes and substrates typically found in fluid dynamics laboratories and identify interesting candidates. We also outline a strategy (ongoing work) how to measure the absorbed amount using fluorescence.

15:30 ***P*** Monitoring the release of mobile oils from burnt food mixtures

Nathan Ravoisin*, Georgina Cuckston and Ian Wilson*
Department of Chemical Engineering and Biotechnology, University of Cambridge, UK

The cleaning of food soils often involves several mechanisms as the soil is frequently multiphase. The aqueous cleaning formulations used in practice include, but are not limited to, surfactants, bleaches and alkali. In studies of cleaning a burnt food soil comprising fats, proteins and carbohydrates, the force required to remove the soils has been measured to change noticeably after an initial period of soaking from an almost constant value to one which decreases exponentially with time. Imaging of the soil layer during the process showed that this transition is related to the liberation of oily species present within the soil.

The rate of oil release from this complex model soil was studied under stagnant conditions. The evolution of oil droplets at the soil-solution interface caused by solubilisation of mobile oil within the soil was monitored by video. Initial results are presented.

15:35 ***P*** Modelling of erosion of thin deposited soils by impinging liquid jets

*Dirk Oevermann, **Ian Wilson**, Rubens Fernandes, Rajesh Bhagat*
Department of Chemical Engineering and Biotechnology, University of Cambridge, UK

We revisit the work of Kaye *et al*. (Investigation of erosion processes as cleaning mechanisms in the the removal of thin deposited soils, *Wear*, 1995, **186-187**, pp. 413-420) on the removal of layers of dried detergent suspension on PMMA plates by impinging water jets, monitored using high speed video. Removal takes the form of an initial breakthrough of the jet to the substrate followed by growth of an irregular, circular area clear of soil. They presented their results in terms of response surfaces, evaluated by statistical fitting to an empirical quadratic model.

We have reanalysed the video records and compare the data with the model for adhesive cleaning by a turbulent liquid jet impinging normally on a soiled, flat plate reported by Bhagat *et al*. (*Food & Bioproducts Processing*, 2017, **102**, 31-54) and show that their model for a 'strong soil' gives a reasonably good description of the data collected by Kaye *et al*. in the Cavendish laboratory 25 years ago.

15:40 ***P*** Modelling of coupled deformation of viscoplastic layers and fluid dynamic gauging flows using two-phase CFD

***Jheng-Han Tsai**, Bart Hallmark and Ian Wilson*
Department of Chemical Engineering and Biotechnology, University of Cambridge, UK

The technique of fluid dynamic gauging (FDG) has been developed to measure the thickness and strength of soft solid layers immersed in a liquid environment, in real time and in situ. FDG measurements involve inducing a small flow into or out of a nozzle located near the surface of the layer. The location of the layer surface (and thus the layer thickness) can be established from the relationship between the measured pressure drop across the nozzle and the mass flow rate.

If the layer material is viscoelastic or viscoplastic the shear stress created by the flow can make the soft layer deform and affect the accuracy of the FDG measurement. Alternately, the absence and then presence of deformation can be used to estimate the yield stress or other characteristic parameter of the material. Here we conduct two-phase computational fluid dynamics (CFD) modelling using the open source software OpenFOAM to predict the deformation of viscoplastic materials during FDG measurement.

The simulation results are compared with experimental data obtained using water as gauging fluid and layers of a commercial petroleum jelly spread across flat substrates. The layer topography is determined using a confocal thickness sensor. When the shear stress exerted by the flow surpassed the layer's yield stress, deformation occurred within one second and did not change thereafter. Good agreement between experimental and simulation data was obtained, indicating that the tool can be used to estimate material yield stresses with some confidence. The results also demonstrated that in suction mode, the shape of crater depends on the breakage.

EXTENDED AFTERNOON BREAK AND POSTER SESSION

16:20 The development and initial testing of the ice pig cleaning method for nuclear reprocessing plants

***Alex Jenkins**, Joe Quarini and Dan McBryde*
Sellafield Ltd, Seascale, UK
University of Bristol, UK

There are numerous situations throughout the nuclear industry where it would be advantageous to clean out enclosed systems, *e.g.* ducts and pipes, to remove sediments and radioactive contamination. However, conventional flushing methods result in the production of significant volumes of contaminated liquor. The wall shear achieved with water flushing is insufficient to remove and carry dense deposits often found in nuclear facilities. Conventional mechanical pigs can be propelled through the duct by application of a driving medium such as compressed air or water. These are able to achieve very high wall shear, but can also get stuck where there is variation in the pipe/duct diameter or small radius bends. The field of application is best suited to straight constant diameter systems with no discontinuities such as T-pieces, valves and in-pipe instrumentation.

Driven by the desire to clean and displace radioactive materials from complex topology ducts and pipes, without the risk of having conventional pigs becoming lodged in a plant and coupled with the need to minimize effluent volumes, the UK Nuclear Industry led by Sellafield Ltd (on behalf of the UK Nuclear Decommissioning Authority), has worked to demonstrate and underpin the use of the ice pigging technology for the nuclear industry.

It is found that high ice fraction slurries flow as viscous liquids that exhibit a number of mechanical properties that offer much higher shear rates. The ‘Ice Pig’ exerts shear rates on pipe walls which are typically 1000 times greater than those achieved with water flowing at the same velocity. The ’Ice Pig’ is able to negotiate almost any topology, flow through pipe networks of vastly differing diameter, through heat exchangers and in-line instrumentation etc.

Experimental data and operational experience from other industries demonstrates that whilst there is high shear, the ‘Ice Pig’ does not damage the surface of the pipe wall. A further attractive characteristic of the ‘Ice Pig’ is that it eventually melts rendering it a simple effluent for processing by downstream processes. Due to the special nature of ice slurry, its unique rheological and physical characteristics, together with the complementary underpinning experimental work undertaken by Sellafield Ltd enables the Ice Pigging process to move from an ‘interesting’ technology to one suitable for use by the nuclear industry for operations, Post Operational Clean Out (POCO) and decommissioning. Furthermore, Ice Pigging has application in many other non-nuclear industries.

16:40 Experimental study of displacement of a Newtonian fluid by shear-thinning solutions

Evangelina Roumpea *and Panagiota Angeli*
Department of Chemical Engineering, University College London, UK

Displacement of a fluid by another that has different properties has found several industrial applications in for example enhanced oil recovery, food industry and pollution spreading. In most of these applications non-Newtonian fluids are used, but there are few studies in the literature regarding the displacement of non-Newtonian fluids. In this project we study the displacement of a Newtonian liquid by a non-Newtonian shear-thinning fluid in a small circular channel.

A low viscosity silicone oil (5 cSt) is used as the Newtonian phase while different concentrations of xanthan gum solutions (1000 ppm and 2000 ppm) are the non-Newtonian fluids. Experiments were conducted at different combinations of flow rates of the two fluids (from 0.01 to 0.1 cm^3/min) and two main flow patterns, namely plug and parallel flow, were observed. Measurements were also carried out with the corresponding Newtonian aqueous solution for comparison. A two-colour Particle Image Velocimetry technique was used to obtain the velocity profiles and shear rates in both phases under different fluid flowrates.

The shear-thinning viscosity was found to produce a more stable flow (constant and uniform displacement of oil) for a large range of flowrates of both phases. With increasing amount of xanthan gum in the aqueous phase, both the velocity of the oil phase and the aqueous film thickness around the oil phase were increased leading to faster displacement of the silicone oil compared to flows without polymer.

17:00 Three-dimensional DNS of product changeover

Lyes Kahouadji*, A. Karnik, L.R. Mason, Richard Craster and Omar Matar*
Department of Chemical Engineering, Imperial College London, UK
Department of Mathematics, Imperial College London, UK

Cleaning of pipes by pushing one fluid through another occurs in a wide variety of industrial applications and has important financial and environmental consequences. The effect of fluid properties (density, viscosity, *etc.*) as well as flow regime (laminar/turbulent) are studied numerically for horizontal pipe geometries. The volume fraction of the original pipe fluid is used as a key indicator for the effectiveness of the cleaning process. The study also extends to more complex geometrical configurations (U-bent pipes, static mixers, *etc.*).

17:20 Using electricalresistance tomography (ERT) to monitor the removal of a non-Newtonian soil by water from a cleaning-in-place (CIP) circuit containing different pipe geometries

***Peter Martin**, Roger Hou, Hassan Uppal and Adam Kowalski*

School of Chemical Engineering and Analytical Science, University of Manchester, UK

Unilever R&D, Port Sunlight Laboratory, UK

Electrical Resistance Tomography (ERT) is used to monitor water based cleaning-in-place (CIP) processes. Specially designed 1.5" transparent Perspex pipes of different geometries, fitted with multiple planes of inline ERT probes, were filled with a non-Newtonian shampoo product, and then cleaned by flushing fresh tap water through at different flow rates ranging from 4000 to 8000 kg/h. The maximum pixel conductivity, defined as the maximum of the reconstructed 316 pixel conductivities in each ERT frame, was proved to be a sound and robust cleaning process monitoring indicator. The investigation demonstrated that the ERT technology is capable of shedding more detailed insights into the CIP process than any other monitoring technologies currently being employed.

17:40 Use of machine learning algorithms for prediction of cleaning efficiency of product changeover process

***Aditya Karnik**, I. Pan, L.R. Mason, Lyes Kahouadji and Omar Matar*

Department of Chemical Engineering, Imperial College London, UK

It is common practice to use a flushing fluid to clean pipelines. At times this technique it used to flush out a resident fluid. This is typical in the fast-moving consumer goods industry when switching the use of a process setup from one product to another. The efficiency of the flushing process is characterised by the amount of resident fluid removed, the ideal scenario being complete removal of the resident fluid. The key parameters affecting such a process are the viscosity ratio of the flushing and resident fluids, and the Reynolds number of the flushing fluid. It is typical to use the Reynolds numbers of the flushing fluid in the turbulent regime to ensure efficient cleaning. In this study, we frame this as a binary classification problem and identify the critical Reynolds number crossover line required to totally remove the resident fluid for a given viscosity ratio by using different machine learning (ML) classifiers employing artificial neural networks, Gaussian processes *etc*.

The geometry is a pipe with two elbow bends representative of the complexity of real-world applications. The classifier is trained by running a set of simulations for different Reynolds numbers and viscosity ratios. Simulations are run until the amount of resident fluid trapped in the pipeline reaches a steady state. For each case, the degree of steady pipe ‘cleanliness’ is based on the presence or absence of resident fluid remaining in the pipeline. The trained ML classifier is then able to predict the outcome of a flushing process for unseen input parameters it has not been trained with. The advantage is the ability of the ML algorithm to learn from a smaller dataset and then predict over the whole parameter space. The novel aspect of this study is the use of artificial intelligence techniques to guide reliable predictions for complex multiphase flows.

9:00 ***Plenary Lecture C***

What a fluid mechanistic needs to know about surfactants

Stuart Clarke

Department of Chemistry/bp Institute, University of Cambridge, UK

What role can and do surfactants (surface active agents) play in cleaning and decontamination? Surfactants can be adsorbed at solution/air interfaces (giving rise to the surface tension phenomena familiar to many fluid mechanicists). They can can also adsorb at substrate /solution interfaces, which together with surface tension determines contact angles and wetting behaviour. They can also adsorb on at soil/substrate, soil/solution and soil/air interfaces, and so it would appear that surfactants play a critical role in this field. In this lecture I will provide an overview about the role surfacants can play and mention some of our work in this area.

10:00 Methods of monitoring cleaning in situ

Georgina Cuckston

Department of Chemical Engineering and Biotechnology, University of Cambridge, UK

Four techniques were used to monitor the mechanisms controlling cleaning of a complex fat, protein and carbohydrate soil mixture from stainless steel substrates. Cleaning was first studied using a modified version of the millimanipulation device described by Magens *et al*. (2017, *J. Food Eng*., **197**, pp.48-59). The device measures the force imposed on a blade which passes through the soil layer at a set translation velocity, in a similar manner to a scraping blade. The modification allowed the flow of cleaning solution across the test sample, at controlled flow rate and temperature, so that the effect of contact time with the solution could be studied. Secondly, the rate of a key component release from the soil was studied in separate tests using stagnant solutions. Finally, the extent of swelling, which is known to affect cleaning, was determined in situ using fluid dynamic gauging and compared to a commercial confocal thickness measurement device. The impact of temperature and pH was studied on each technique.

At raised temperatures the force required to remove the deposit changed noticeably after a given soaking time from an almost constant value to one which decayed almost exponentially with time. The critical soaking time depended on both the temperature and pH of the cleaning solution and in many cases was associated with a transition from cohesive to adhesive breakdown. The critical soaking time matched well with critical times found in swelling testing and release of the key component.

10:20 Experimental study of the removal of bulk contaminant droplets using an ionic liquid simulant

Merlin Etzold *and Stephen Marriott*

Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK

Defence Science and Technology Laboratory (DSTL), UK

Well-defined laboratory experiments can provide fundamental insight into the physics of decontamination but require model contaminants (simulants), whose properties are sufficiently close to the real contaminants under consideration without posing environmental and safety hazards. We demonstrate the use of an ionic liquid developed by DSTL as simulant in experiments modelling bulk-removal of chemical weapon droplets from the bottom of small gaps and cracks. In highly concentrated from, the ionic liquid is a red oil which easily wets glass surfaces, whilst in diluted form it behaves like a fluorescent dye. We explored these properties to conduct droplet-washing experiments in a rectangular glass geometry. Depending on the Reynolds number, we observed either dissolution of an essentially geometrically unchanged droplet, deformation of the droplet leading to the formation of a corner flow or erosion due to shear forces.

We discuss the occurrence of these regimes and discuss modelling of the dissolution regime using a boundary layer model, assuming a first-order dissolution process at the boundary.

MORNING BREAK

10:40 Drop dynamics on liquid infused surfaces

Halim Kusumaatmaja, *Muhammad Sadullah, Alvin Shek and Ciro Semprebon*
University of Durham, UK
Northumbria University, Newcastle-upon-Tyne, UK

Inspired by pitcher plants, the so-called liquid infused surfaces (LIS) are constructed by infusing rough or porous materials with a lubricant. They exhibit many advantageous surface properties, including self-cleaning, drag reduction, and anti-fouling; and as such, they are favourable for applications to a wide-range of problems, ranging from marine fouling and product packaging to heat exchanger and medical devices.

In this contribution, we will focus on two interesting aspects when a droplet is placed on LIS. First, the main distinguishing feature of LIS is the presence of the lubricant, which forms a ridge surrounding the droplet. We show that the apparent contact angle is not uniquely defined by material parameters, but also has a dependence on the relative size between the droplet and its surrounding wetting ridge. Numerical simulations further reveal a rich interplay between contact line pinning and viscous dissipation at the lubricant ridge as a droplet moves across LIS. Secondly, we simulate the behaviour of a capillary bridge sandwiched between two LIS, and quantify the force and maximum separation distance before the capillary bridge breaks up. Interestingly, for LIS, we find the capillary forces are stronger and the capillary bridge can be stretched further, when compared to the standard case of a capillary bridge between two smooth homogenous surfaces. Thus, we can effectively have a substrate which is slippery in one direction, but sticky in another direction.

11:20 Experimental derivation of chemical evaporation rates from unclothed and clothed sebum-coated discs under various exposure conditions.

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University of Hertfordshire, UK

The rate and extent of chemical evaporation from clothing or exposed skin surfaces may affect the efficacy of decontamination by influencing the amount of chemical available.

For instance, lower volatility compounds are amenable to skin decontamination for longer durations than highly volatile chemicals. Consequently, the ability to predict chemical evaporation from clothing and exposed skin surfaces will provide first responders with a means of rapidly identifying an appropriate and proportionate response strategy. The objectives of this study were to measure the rate at which a range of chemicals evaporate from an artificial skin surface and how different droplet volumes and application geometry (single vs. multiple droplets of the same volume) influence evaporative loss in clothed and unclothed exposure scenarios.

Fifty-five chemicals (with a range of physicochemical properties) were applied to aluminium discs coated with a thin (6.8 µm) film of artificial sebum equilibrated to 32ºC, either as single droplets at different doses (2, 10, 15, 20, 40 or 200 µL) or as multiple droplets of the same dose (1×20, 2×10, 4×5, 6×3.33, 8×2.5 and 10×2 µL). Evaporation rates were measured gravimetrically at 15 minute intervals for 1 hour

Rates of evaporation from the sebum and clothed discs were proportional to droplet size, *i.e.*, smaller droplets evaporated faster than larger droplets. The presence of a clothing layer consistently decreased the rate of evaporation. However, there was no statistically significant correlation observed between the rate of evaporative loss from sebum or clothing surfaces and any single physicochemical property of the 55 chemicals.

These data suggest that the process of evaporation from sebum-coated discs is complex and likely to be driven by an interplay of several physicochemical parameters. Work with this comprehensive data set is ongoing to develop a predictive algorithm for use by first responders as part of a decision-aiding tool to identify the most relevant action for casualty management such as no treatment, disrobe only, or disrobe and decontamination.

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11:40 The influence of the thermal properties of the system on the lifetime of an evaporating droplet

Feargus Schofield*, Stephen K. Wilson, David Pritchard and K. Sefiane*
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University of Edinburgh, UK

Understanding the dynamics of sessile liquid droplet evaporation on solid substrates is critical for many industrial processes, such as washing, coating, and ink-jet printing. Through the understanding of droplet evaporation, it is possible to predict, and even control, the deposition patterns left by evaporated solutes. Consequently, in recent years there has been a rapid growth of scientific interest in all aspects of droplet evaporation, including determining the lifetimes of evaporating droplets.

Previous work has shown that the mode in which a droplet evaporates is a key factor in determining the lifetime of an evaporating droplet. However, much of this work uses the standard diffusion-limited model for droplet evaporation. The standard model does not account for other key factors in droplet evaporation, such as the thermal properties of the droplet, substrate or atmosphere. The initial thermal properties of the system have been shown to have a significant influence on the evolution of an evaporating droplet.

In the present work we investigate the influence of the thermal properties of the system on droplet evaporation in order to predict the lifetime of the droplet. In particular, we investigate droplets evaporating on substrates with a relatively low thermal conductivity compared to that of the liquid, such as alcohols on plastics, in each of the constant radius (CA), constant angle (CA), stick-slide (SS) and stick-jump (SJ) modes of evaporation.

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12:00 Numerical simulations of moving contact lines

***Yi Sui**, Hang Ding and Peter DM Spelt,*

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Flows involving moving contact lines (MCLs) are widely found in nature and industry. A major challenge in modelling MCLs is that the conventional hydrodynamic theory combined with a no-slip boundary condition at the wall leads to a non-integrable stress singularity at the contact line.

In this talk, I will first review a few major theoretical models and computational methods for moving contact lines, and the main associated challenges. Then I will introduce a recent computational model for practical simulations of moving contact lines. The model borrows the idea from the large eddy simulation in turbulence modelling; it resolves the macroscale flows only while model the effect of MCLs using modified hydrodynamic theories. Finally, I will briefly cover the recent extension of the simulation tool to non-isothermal systems and some new interesting results.

12:20 Surface permeability and capillary transport

Alex Lukiyanov, T. Pryer and P. Shirimak

University of Reading, UK

We have established previously, in a lead-in study, that the spreading of liquids in particulate porous media at low saturation levels, characteristically less than 10 % of the void space, has very distinctive features in comparison to that at higher saturation levels. In particular, we have found that the dispersion process can be accurately described by a special class of partial differential equations, the super-fast non-linear diffusion equation. The results of mathematical modelling have demonstrated very good agreement with experimental observations. However, any enhancement of the accuracy and predictive power of the model, keeping in mind practical applications, requires the knowledge of the effective surface permeability of the constituent particles, which defines the global, macroscopic permeability of the particulate media. We demonstrate here how this quantity can be determined through the solution of the Laplace-Beltrami Dirichlet problem, we study this using the well-developed surface finite element method, and discuss further applications.

12:40 Gas nanofilms in drop impact and spreading

James Sprittles
Mathematics Institute, University of Warwick, UK

Understanding the outcome of a collision between liquid drops (merge or bounce?) as well their impact and spreading over solid surfaces (splash or spread?) is key for a host of processes ranging from 3D printing to cloud formation. Accurate experimental observation of these phenomena is complex due to the small spatio-temporal scales or interest and, consequently, mathematical modelling and computational simulation become key tools with which to probe such flows.

Experiments show that the gas surrounding the drops can have a key role in the dynamics of impact and wetting, despite the small gas-to-liquid density and viscosity ratios. This is due to the formation of gas nanofilms which exert their influence on drops through strong lubrication forces. In this talk, I will describe how these nanofilms cannot be described by the Navier-Stokes equations and instead require the development of a model based on the kinetic theory of gases. Simulation results obtained using this model will then be discussed and compared to experimental data.

LUNCH

14:00 Homogenisation of agents and cleansers interacting on a microscale

Ellen Luckins *and Chris Breward*
Mathematical Institute, University of Oxford, UK

Abstract not available

14:20 Decontamination in cracks and fractures

Julien Landel*, Merlin Etzold and Stuart Dalziel*
School of Mathematics, University of Manchester, UK
Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK

The decontamination of confined spaces such as the gaps, cracks, pores and folds of materials poses many challenges. When hazardous liquids are spilled over permeable material surfaces, such as most building materials, grounds or porous equipment materials, a portion can be driven into the sub-surface features of the materials through gravity, capillary forces or the initial momentum at impact. Usual decontamination techniques to decontaminate external surfaces, such as spraying a decontaminant over contaminated surfaces, are not effective for sub-surface features. Indeed, the neutralisation of the contaminants works best when the area in contact with the decontaminant is maximised and also when the decontaminant flow is increased. In addition, applying the decontaminant under a pressure jet at the material surface could drive the contaminant further into the matrix of the material without achieving full decontamination. This could also pose a long term exposure risk due to delayed or continuous release of the contaminant over a long time.

In this study, we present modelling results showing the impact of geometrical confinement for the decontamination of a drop lodged inside a U-shape or a V-shape crack. We model the convective mass transfer at the interface of the drop and the decontaminant flow using advective-diffusive boundary layer techniques. We note that neutralisation processes are not modelled in the advection-diffusion governing equations. The effect of the mass transfer is characterised by a Sherwood number which depends on the Péclet number rescaled with the aspect ratio of the drop dimensions. In particular, we find a complex dependence of the Sherwood number with the rescaled Péclet number in the case of V-shape cracks depending on the ratio of the boundary layer thickness and the crack width. Finally, we discuss typical scenarios of the decontamination of drops in cracks compared with drops on flat surfaces. We find that below a certain threshold depending on the rescaled Péclet number the time of decontamination increases significantly in confined spaces.

14:40 Modelling unsaturated decontamination

Oliver Whitehead and Chris Breward
Mathematical Institute, University of Oxford, UK

Abstract not available

15:00 Impinging water jet cleaning of a hydrophobic non-Newtonian soil on flat surfaces

Rubens Rosario Fernandes, Rajesh Bhagat, Bart Hallmark and Ian Wilson
Department of Chemical Engineering and Biotechnology, University of Cambridge, UK

Cleaning-in-place technologies are essential to avoid cross-contamination of products in the food and pharmaceutical industries. This work addresses the removal of viscoplastic soil layers from flat plates using impinging, coherent water jets. The jets are generated using 2 mm nozzles, are turbulent, and impinge normally on the coated surface. A range of jet flow rates are considered. Surfactants were not used.

Layers of petroleum jelly with different thicknesses were coated on Perspex and glass plates. The growth of the cleaned radius over time was described well by the Glover *et al*. (2016, *J. Food Eng*, **178**, 95–109.) model, reaching a maximum cleaned radius which was smaller than the location of the hydraulic jump observed when the jet impinged on the uncoated surface. Additionally, scans of the shape of the craters generated by the jet after different impinging times using a confocal thickness scanner device showed that the profiles of the rims do not follow the wedge shape assumed in the Glover *et al.* (2016) model, but exhibit a range of angles up to 45˚.

The rheology of the jelly was studied using a number of rheometric techniques. Increasing shear stress ramps and steady-state flow curves showed that the static and dynamic yield stresses differ considerably, indicating strongly thixotropic behaviour. A shear-driven model was developed to describe the displacement of the soil by the shear stress generated by the thin liquid film in the radial flow zone. Results are presented for the case of a Bingham fluid: these show that a simple shear-driven erosion model does not provide an adequate description of the cleaning process of these complex fluids.