Roadmapping of Quantitative Understanding and Modelling of Cleaning and Decontamination

List of abstract for the contributed presentations

On Day 1, at 15:00-16:30, all presenters of talks and posters are invited to be in the room indicated for 30 min. Other delegates will be able to come and discuss their presentation with them.

Each presenter also has a room with the link to their presentation available throughout the workshop.

Time	*Presenter*	*Title*	*Talk/Poster*	*Room name*
15:00	Chris Breward	A simple model for desulphurisation of flue gas using reactive filters	T	Breakout 1
15:00	Loïc Chagot	Interfacial instabilities during microchannel cleaning with a viscoelastic fluid	T	Breakout 2
15:00	Francesco P. Contò	Surface-washing of contaminated porous substrates	P	Breakout 3
15:00	Merlin A. Etzold	Hydrogel models to study contaminant trapping in polymers	P	Breakout 4
15:00	Rubens R. Fernandes	Advances and challenges towards a predictive model for cleaning very thin viscoplastic soil layers using impinging liquid jets	T	Lounge A
15:00	Christian Golla	Usability of results from micromanipulation experiments to get critical loads for adhesive and cohesive removal of soils	T	Lounge B
15:30	Halim Kusumaatmaja	Droplet Dynamics on Liquid Infused Surfaces	T	Breakout 1
15:30	Brent A. Mantooth	Characterizing Hazard Mitigation Efficacy for Different Agent Distributions	P	Breakout 2
15:30	Abhinav Naga	How a water drop removes a particle from a hydrophobic surface	T	Breakout 3
15:30	Siddharth V. Patwardhan	Bioinspired nanomaterials for environmental decontamination	T	Breakout 4
15:30	Thomas P. Pearl	Roles of surface wetting and bulk mass transport in the contamination of polyurethane-based coatings by distilled mustard blister agent, HD	P	Lounge A
16:00	David Fernandez Rivas	Cleaning in a bag	T	Breakout 1
16:00	Mark J. Varady	Development and Application of Model for Decontamination of Polymer-Based Materials	P	Breakout 2
16:00	Nik Watson	Robots, Sensors and Artificial Intelligence: How can digital technologies improve cleaning processes?	T	Breakout 3
16:00	Jialiang Yin	Concept for a self-learning adaptive tank cleaning strategy	P	Breakout 4
16:00	William B Zimmerman	Cleaning by microbubbles generated by fluidic oscillation with and without plasma injection	T	Lounge A

A simple model for desulphurisation of flue gas using reactive filters

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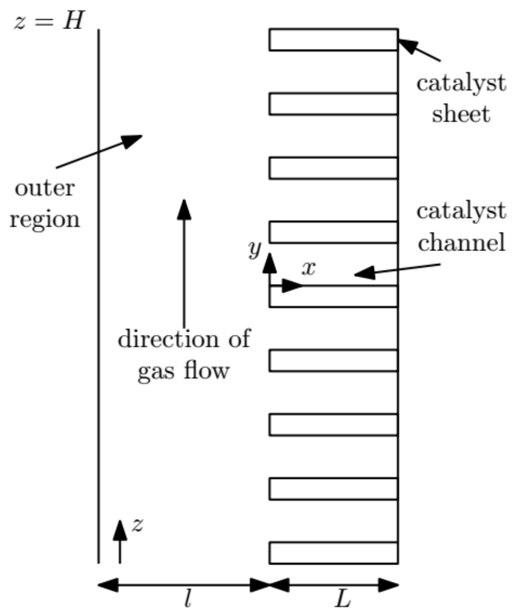
Presentation: Talk

Desulphurisation of flue gas is essential before it can be released safely into the atmosphere. One way of removing sulphur dioxide is to use a purification device incorporating a reactive filter, in which the flue gas stream passes in front of a porous-catalyst-filled structure which converts the gaseous sulphur dioxide into liquid sulphuric acid. In this talk, we will present and solve a simple mathematical model [1] to describe the operation of a paradigm reactive filter. Our model incorporates the transport of sulphur dioxide through the device via advection in the main “outer” flow, diffusion through the catalyst structure, and the production of sulphuric acid, which gradually accumulates in the filter rendering it less efficient.



We will explore how the key parameters governing the device affect the efficiency.

Acknowledgements:

We are very grateful for many useful conversations with Ian Griffiths (Oxford University), Don Schwendeman (Rensselaer Polytechnic Institute), Uwe Beuscher (W. L. Gore and Associates, Inc.), and Vasu Venkateshwaran (W. L. Gore and Associates, Inc.). This work was partially supported by a summer placement grant by Christ Church, Oxford, and by the EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling (EP/L015803/1).

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Interfacial instabilities during microchannel cleaning with a viscoelastic fluid

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Presentation: Talk

Knowledge of the behaviour and characteristics of immiscible displacements in microfluidic devices is critical to optimize their cleaning process. The displacement of a liquid by another fluid has been studied extensively during the last decades. As shown by Saffman and Taylor (1958) [1] for porous media and Hele-Shaw cells, when a viscous liquid is pushed by a less viscous one, the interface between them tends to become unstable. This instability often leads to inefficient cleaning as a liquid film remains trapped at the wall. The observations can be extended to microfluidic displacements and many experimental studies have been performed for Newtonian flows ([2], [3]). For non-Newtonian flows, Gan et al. (2007) [4] highlighted that viscoelastic flow instabilities can promote a more effective mixing than in viscous/viscous or viscous/inertial fluid configurations. However, the impact of the viscoelastic properties of complex fluids on the space-time scales of these instabilities is still poorly understood.

In the present study, interfacial instabilities were investigated during the displacement of a silicon oil by a viscoelastic aqueous solutions using interface tracking. The aqueous phase was a Boger fluid comprising of a mixture of polyethylene glycol (PEG), zinc chloride (ZnCl2) and polyethylene oxide (PEO). For reference, experiments were also carried out with a Newtonian aqueous solution (PEG + ZnCl2). The density and viscosity ratios of the two immiscible fluids were the same in both cases.

The experiments were performed in a glass circular microchannel with a diameter of 200 microns. To capture the dynamic of the interfacial instabilities, images were taken with a 12 bit high-speed camera with 1280 x 800 pixels resolution equipped with a microscope lens (50x). A backlight system using LED ensured a homogeneous illumination of the micro-channel. To allow full optical access and avoid optical distortions, in particular close to the wall, the solutions were selected to have refractive index that matches that of the microchannel glass. Moreover, this setup allows to investigate velocity fields using 2D micro Particle Shadow Velocimetry (µPSV) with 1 µm polystyrene particles.

The results showed that interfacial instabilities appear earlier for the viscoelastic fluid than the Newtonian one. Moreover, the amplitude of the interfacial deformation is larger for the Boger fluid, which can be a key parameter to control the cleaning efficiency in microfluidic devices. The results will be linked to the velocity fields to quantify the local effects at the interface.

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Surface-washing of contaminated porous substrates

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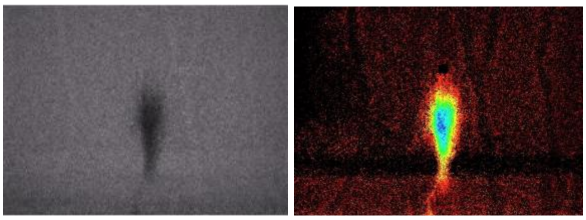
Presentation: Poster

The cleaning of porous surfaces is a challenging problem in everyday life and industrial practice since it can lead to a redistribution of the absorbed contaminant within the porous material instead of a complete removal of the unwanted agent [1]. In this work, we present surface-washing experiments modelling the decontamination of porous substrates.
Firstly, we report a protocol to manufacture mechanically stable porous media by sintering glass ballotini (< 1 mm) to form free-standing homogeneous porous plates or composite structures where a porous matrix is sintered onto solid glass backing and surrounds. The ability to incorporate directly a solid glass backing provides a method of preventing any liquid leaks through their rear. These samples are then integrated into an apparatus used in a previous work which studied surface-washing decontamination of impermeable surfaces [2].
A dyed fluid is placed onto the porous substrate to simulate the region of contamination. The surface-washing is simulated by a thin (~1 mm) film of water flowing from a reservoir through a gap over an inclined porous-glass surface. The resulting interaction between the cleansing film flow and the contaminating dye is then tracked using dye attenuation, enabling us to analyse the contaminant field in space and time.
Our experiments provide insights on the role of initial conditions (wet/dry substrate), the impact of cleaning strategies on industrial performances (e.g., decontamination time), and the relevant transport mechanisms of the contaminant (gravity or capillary advection and diffusion in both water and porous medium). Importantly, they demonstrate a decontamination-induced redistribution of the contaminant within the porous matrix.



A porous surface contaminated with a 1 ml droplet of 0.01% methylene blue is washed by a water film. Left: grey scale image; Right: colour map of the contaminant concentration.

Acknowledgements: The authors acknowledge "Dstl" (UK) as the main sponsor of the work.

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Hydrogel models to study contaminant trapping in polymers

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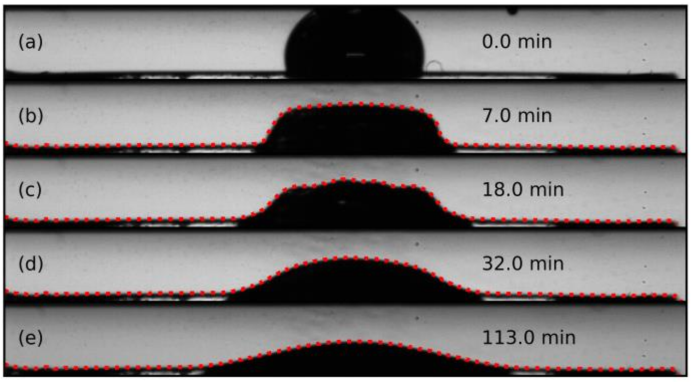
Presentation: Poster



Absorption of a single contaminant droplet into a high-swelling polymer

Some cross-linked polymers, such as hydrogels, can absorb large quantities of solvents whilst undergoing a large change in volume. Such processes can trap hazardous contaminants, hinder decontamination and pose a long-term hazard to humans and the environment. Such processes are hard to study in many practically relevant systems due to difficult flow diagnostic within the solid.

In our experiment we circumvent this problem by choosing an extremely high-swelling polymer, a medical grade hydrogel. In this system, water acts as contaminant. We place a single droplet of contaminant on a thin layer of polymer. Within minutes, a strongly swollen, localised blister with a patterned surface forms. Over the next few hours, the pattern vanishes and the blister spreads radially whilst significant swelling remains.

We experimentally show that this process is driven by transport of solvent within the polymer and within the vapour contained in the surrounding gas phase. We also show how these two transport phenomena can be experimentally separated to enable the study of the transport within the polymer alone. The long-time dynamics of transport within the polymer is compared against two linear poroelastic models which agree well with the observed kinetics and blister shape.

Acknowledgements: MAE, JRL and SBD acknowledge funding from Dstl

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Advances and challenges towards a predictive model for cleaning very thin viscoplastic soil layers using impinging liquid jets

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Presentation: Talk

Impinging liquid jets are widely employed on the cleaning and decontamination of soiled surfaces in the food, FMCG and pharmaceutical industries. When the liquid jet impinges on a surface, it spreads radially outwards from the point of impingement as a thin liquid film. If the surface is soiled, this liquid film is responsible for cleaning. Yeckel and Middleman [1] modelled the case when a very thin layer of a Newtonian oil is cleaned by a spreading water film. They assumed that the Reynolds' lubrication approximation holds for the flow in the soil layer and described the progressive shear-driven removal of the soil layer over time. Recent works [2-4] have described the cleaning of thin viscoplastic soil layers, when the soiling material does not flow unless a critical shear stress is surpassed. These models assume that a momentum-driven mechanism is responsible for cleaning, meaning that the soil is pushed outwards by the radially expanding liquid film. However, experimental observations [3,4] indicated that the dynamics of the cleaning of very thin soil layers (when the liquid film flows above the soil layer instead of being deflected by it) differs from the thin layer case.

In this talk, we will present a shear-driven model to describe the removal of very thin layers of a petroleum jelly by coherent turbulent impinging water jets. The rheology of the soil was investigated by rotational rheometry and displayed strong time-dependent behaviour. The Yeckel and Middleman [1] model was adapted to account for the cleaning of a very thin Herschel-Bulkley soil and failed to provide an adequate description of the evolution of the cleaned region. An energetic analysis indicated that this does not result from the uncoupling between the flows in the liquid film and in the soil layer, but rather from a simple yield stress material description not being sufficient to describe the rheology of the soil. The challenges to obtain a fully predictive model for the cleaning of very thin viscoplastic soil layers will also be discussed.

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Usability of results from micromanipulation experiments to get critical loads for adhesive and cohesive removal of soils

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Presentation: Talk

In terms of food safety, regular cleaning is an important process step. Machine equipment in the food industry is cleaned almost daily and therefore causes high economic and ecological expenses. Predicting the cleaning time required to remove a thin layer of soil is a challenging task and subject of current research.
The authors recently presented a model for the cleaning mechanism of adhesive detachment and validated it successfully with ketchup in a fully developed channel flow and a channel flow with sudden expansion. In this presentation, the existing model is extended for the modelling of cohesively separating soil layers. For this, the cohesive binding forces are determined in millimanipulation experiments. However, the load application within those experiments differs from the cleaning experiments. This talk presents the current work status to this issue. The authors hope to benefit from the discussion with experts present in the field of cleaning. Since the modelling approach is the same as for the adhesively detaching soils, transitions between these cleaning mechanisms will be possible to simulate with the corresponding parametrization in the future.

Droplet Dynamics on Liquid Infused Surfaces

Halim Kusumaatmaja[a]*, Muhammad S. Sadullah[a], Jack R Panter[a], Ciro Semprebon[b]

Presentation: Talk

Inspired by pitcher plants, a novel class of functional surfaces, termed liquid infused surfaces (LIS), can be constructed by infusing rough or porous materials with a lubricant [1,2]. They have been shown to exhibit a wide range of advantageous surface properties, including self-cleaning, drag reduction, anti-icing and anti-fouling. In this contribution I will present our recent lattice Boltzmann simulation results studying the motion of deposited droplets on LIS. First, I will discuss the rich interplay between contact line pinning and viscous dissipation at the lubricant ridge around the moving droplet, which become dominant at large and small apparent angles respectively [3]. Second, I will discuss the pinning force experienced by the droplet when partially wetting lubricants are used, which depends on the solid fraction, the lubricant wetting angles, and the various fluid surface tensions [4].

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Characterizing Hazard Mitigation Efficacy for Different Agent Distributions

Brent A. Mantooth, Thomas P. Pearl, Neil Hawbaker, Janlyn Eikenberg, Mark J. Varady

Presentation: Poster

Hazard mitigation technologies are used to reduce the exposure for personnel who interact with contaminated objects. The ability to remove agent from a material is dependent on the distribution of the agent on or in the material, including absorbed, surface adhered, and capillary entrained liquids. Agent distributions can be generated and affected by different rate limiting mechanisms, and these processes influence the exposure to personnel and the efficacy of decontamination technologies for agent removal. Testing for decontamination efficacy must rely on materials-level, lab-scale tests. Therefore, specific agent distributions are created in laboratory testing to isolate and characterize the mechanisms of removal. The ability to bridge the gap from laboratory to field use depends on accounting for how these mechanisms contribute to removing the agent from each distribution. New laboratory methods are presented that explore how to generate specific agent distributions, to characterize decontamination efficacy, and to evaluate how these different distributions contribute to personnel exposure.

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How a water drop removes a particle from a hydrophobic surface

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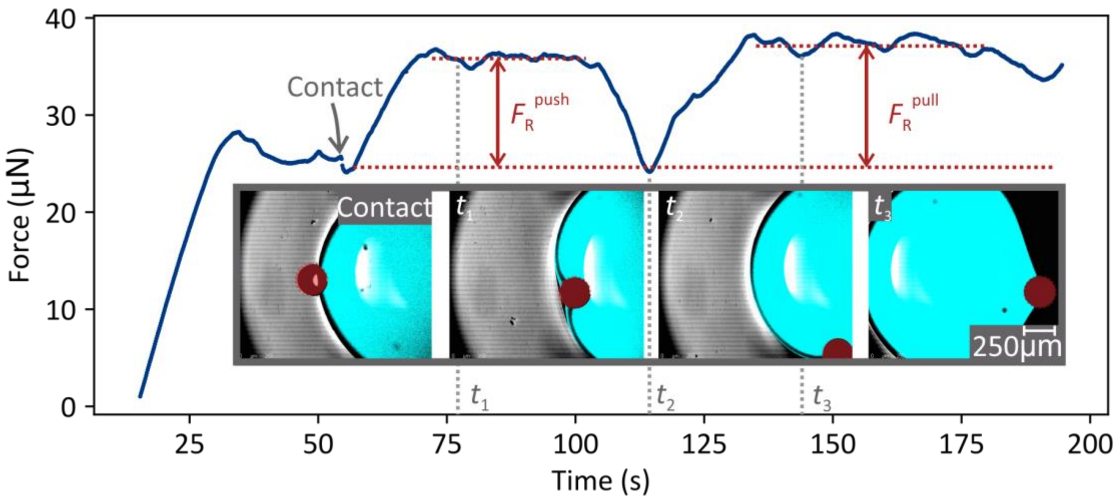
Presentation: Talk

The contamination of surfaces by dirt particles is problematic in many applications. To contribute to solving this problem, we investigated how a drop removes a particle from a surface. So far, there is no study focussing on a single-particle level. Here, we address the following questions: How does the collision between a drop and a single particle look like on a microscopic scale? Which forces determine whether a particle can be removed?

We used an inverted confocal microscope to study the removal of particles from a hydrophobic surface by a water drop [1]. The drop was held at a fixed position by a blade, while the particle was moved at constant speed towards the drop. This setup allows to image the drop-particle collision and to measure the force acting on the drop during the collision. Different outcomes are observed, depending on the speed of the collision. At low speeds, the particle remains attached to the drop (as shown in the figure below) whereas, at high speeds, the particle enters and exits the drop.

Particle removal is possible when the maximum capillary force that the drop can exert on the particle is greater than the resistive force experienced by the particle. Both the capillary and resistive forces depend on the geometry of the particle, its surface properties, and how it moves (whether it rolls or slides) over the surface. We discuss the contributions to the resistive forces and derive analytical expressions for the maximum capillary force that the drop can exert on a rolling and a sliding particle. Particle removal can be enhanced by lowering the resistive force.



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Selected as 'Soft Matter hot article': a short blog article is available here.

Bioinspired nanomaterials for environmental decontamination

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Presentation: Talk

Porous materials such as silica, carbons, metal organic framework materials, porous polymers and others, are used in a variety of environmental decontamination applications. However, these materials are generally prepared under environmentally damaging conditions, leading to secondary pollution – this only shifts the pollution problem. Taking inspiration from organisms and understanding the molecular principles in biomineralisation, we have developed green nanomaterials (GN) synthesis,[1] which offers substantial reductions in resources, time, energy usage and costs, yet producing high value materials.

This presentation will show how we have demonstrated the utility of GN in environmental decontamination by combining experiments and modelling. GN exhibited very high extraction efficiencies for a range of VOCs including formaldehyde[2] and monoaromatic hydrocarbons (e.g. benzene, toluene and cumene).[3] Upon modelling their porosity, it was observed that the combination of broad pore size distribution, disordered arrangement of pores and the presence of meso- and micro-porosity in GN contributed to their extraction efficiencies and selectivity.

Through a systematic approach, the removal of anthraquinone dyes from water showed up to 94% removal when using GN and the highest adsorption capacity compared to literature example.[4] Examination of the effects of various adsorption conditions and modelling the kinetics and isotherms helped reveal the removal mechanisms. For As removal, for the first time, a family of iron supported on GN was prepared,[5] which exhibited high extraction efficiencies, high adsorption capacities and superior kinetics (threefold higher than the highest removal rates reported to date). Moreover, a method was developed to regenerate GN allowing for full recovery and reuse of the adsorbent in subsequent extractions; strongly highlighting the potential technological benefits of these new green materials.

In summary, GN have excellent performance, good thermal stability and a reuse potential, with a substantial reduction in secondary pollution – they form a viable alternative to traditional porous materials in environmental decontamination.

Acknowledgements: This abstract summarises work conducted by various researchers in our group over past 5-7 years in collaboration with Dr. Lorraine Gibson (University of Strathclyde) and other colleagues noted in the references below.

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Roles of surface wetting and bulk mass transport in the contamination of polyurethane-based coatings by distilled mustard blister agent, HD

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Presentation: Poster

This work focuses on determining physicochemical interactions that influence the resistance of materials to chemical contamination, specifically for the case of a liquid phase chemical warfare agent exposed to polymer composite materials. The degree and type of retention is a function of wetting behavior at the surface as well as the propensity for penetration of the liquid phase into bulk layers of the exposed material. Experimental work has been performed to study the interaction of distilled mustard blister agent, HD (bis(2-chloroethyl) sulfide), with polyurethane-based, low reflectivity coatings, which can be treated as high solids loaded polymer composites. Results elucidate entrainment in near-surface capillary networks and transport into bulk layers through molecular diffusion as a function of variations in polymer binder and solids loading in the composite. The understanding garnered from considering chemical retention informs next generation decontamination approaches as well as new coatings formulations that are tuned for chemical resistance, reduced decontamination burden, and mitigated hazard for Warfighter personnel. Approved for public release: distribution unlimited.

Cleaning in a bag

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Presentation: Recorded-talk

Ultrasonic cleaning relies on bubbles collapsing in the vicinity of the contaminated substrate, and different physical mechanisms involved when bubbles collapse have been discussed [1]. Cleaning processes are enhanced by controlling the location where bubbles appear, influencing the cavitation nucleation process. Artificial microscopic pits act as source of ultrasonic cavitation nuclei [2] and can be used for cleaning small areas on flat substrates [3]. Numbering up the pits, a three-dimensional way to increase the desired effects of cavitation in a controlled way was named Cavitation Intensifying Bags (CIB), commercialised as BuBble Bags (www.bubclean.nl). CIB have demonstrated the potential to improve reproducibility and enhance processes such as cleaning larger and arbitrary objects, and sonochemistry [4-8]. Our team has also developed methods to quantify cleaning [9-11], and more fundamental studies of bubbles collapsing near complex geometries [12].

*The author is co-founder of BuBclean and receives no financial compensation.

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Development and Application of Model for Decontamination of Polymer-Based Materials

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Presentation: Poster

The ability to predict decontaminant performance fills critical gaps in testing since (1) it is often not possible to test over all operational conditions of interest, and (2) accurate models can provide insights into the mechanism of action and how modifying process parameters influences performance. To accomplish this, our model simulates all the physical and chemical processes that occur from the time a liquid agent droplet contacts the asset, through decontamination, and after the decontaminant is removed. For military coatings, the transport processes on the surface and in the bulk of the material are complex due to the irregular and heterogeneous nature of the material. This required development of high fidelity models for surface liquid spreading and diffusion in polymer-based materials to ensure accurate prediction. The process of designing experiments to obtain the necessary model parameters is described along with specific case studies varying the operating conditions and exploring scenarios not yet tested in the laboratory. Some examples include examining variations in the decontaminant thickness and timing of the decontamination process.

Acknowledgements: This research was funded and supported by the Defense Threat Reduction Agency (DTRA)/Joint Science and Technology Office (JSTO) under project CB3062. We thank the Decontamination Sciences Branch for their hard work and expertise that greatly assisted with the execution of this research project. The views expressed in this abstract are those of the authors and do not necessarily reflect the official policy or position of the Department of Defense or the U.S. Government.

Robots, Sensors and Artificial Intelligence: How can digital technologies improve cleaning processes?

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Presentation: Talk

Digital technologies such as robots, sensors and machine learning are impacting all aspects of our lives but how can they be applied to cleaning and disinfection processes within industrial and public environments?
This talk will provide an update on a number of current research projects at the University on Nottingham exploring within this area including:

- Ultrasonic sensors and machine learning to monitor clean-in-place processes
- Ultraviolet cleaning robots for space disinfection
- Effective human robot interaction for industrial cleaning

The talk will briefly cover the technical aspects of these technologies whilst also focussing on the areas of trust and user acceptability, essential for widespread adoption.

Concept for a self-learning adaptive tank cleaning strategy

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Presentation: Poster

We are introducing an approach with an adaptive, self-learning strategy to reduce failures and resource consumption of CIP-processes using tank cleaning as an example. We are planning to monitor the contamination status inside the tank inline by means of optical sensors and to model the correlation between process parameters and cleaning result [1]. Based on this model and the current process status, an optimization for searching new best parameters can be proposed. Using a conventional way, this correlation could be modelled physically and represented by a multidimensional function using expert knowledge. Still, this modelling is cumbersome and error-prone as many parameters have to be considered. We follow the approach to build the correlations in a black box model using data-driven modelling techniques like machine learning with data collected from cleaning processes in laboratory to map process parameters and current cleaning status onto cleaning results and efficiency [2], [3]. According to the Sinner Circle, four main factors are influencing the cleaning process: mechanical and chemical action, the temperature of the cleaning fluid as well as cleaning duration. Other parameters, for instance the type of product and its conditions, have to be considered for modelling as well. Using those input parameters and cleaning result, a mapping regression function can be created to represent the cleaning process.

Once the model is obtained, we are able to calculate the resulting resource costs, such like energy, for the set parameters, e.g., water flow and pressure, and the resulting cleaning success. It is then possible to search for extreme values and find out the parameters leading to these extrema. To achieve the extrema, firstly a cost-fitness function must be introduced to calculate the complete cost of the process based on variable set and fixed parameters. Here meta-heuristic algorithms will be applied to estimate those values [4]. Running this new set of parameters after optimization, a new dataset for the machine learning model can be created to relearn and thus the machine learning model can be improved.

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Cleaning by microbubbles generated by fluidic oscillation with and without plasma injection

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Presentation: Talk

Microbubbles generated by fluidic oscillation are unique in that they require so little power that they can maintain laminar flow. Laminar flow, it turns out, is actually very good at cleaning, as it can create very strong wall shearing forces. The flow in the lubrication layer between microbubbles and surface, either impingent or transverse motion, squeezes and thus scours efficiently. In this oral presentation (recorded), microbubbles are observed to maintain clean surfaces in bioprocesses [1], so are explored for how fast and how effectively they can remove biofilms. Confocal images show >99% removal in 3 minutes of contact time, against the industrial benchmark of 1hr and 90% removal effectiveness.

Separately, microbubbles can be the agent for delivering plasma activated ionized gas to liquid media, by a novel injection system where the diffuser also serves as an electrode (see Figure 1). This configuration achieves the same ozone generation rate as our earlier dosing lance, but draws 5W vs. 130W power for its predecessor, which achieved a 5-log disinfection in a pilot plant trial on final effluent, treating 1L/min. There are no published benchmarks for commercial performance, but anecdotally, 750W is ordinarily required for such treatment rates. Although ozone is commonly used for this purpose, because the output of the plasma reactor is the input to the microbubble, excited species generate hydroxyl radicals on contact with microbubble interface, bypassing the known bottlenecks of ozone dispersal, dissolution, and dissociation (into hydroxyl radicals) that are all slow steps

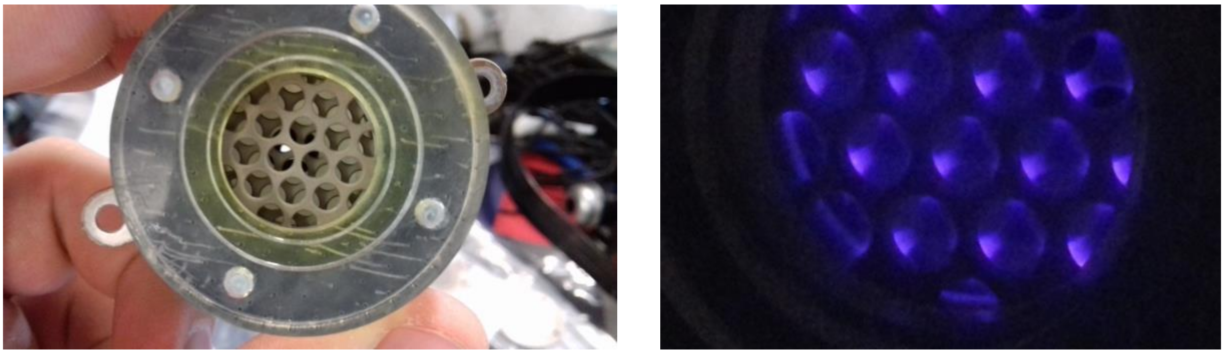

Figure 1 Plasma microbubble injector (left) with diffuser serving as second electrode; (right) ultraviolet light as plasma is excited (courtesy of Dr Tom Holmes).

Acknowledgements
EPSRC, NBIC, Perlemax. Dr Tom Holmes, Dr Pratik Desai, Dr Joy Mukherjee

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