



EPSRC Workshop Grant EP/T033991/1

A Roadmap for Quantitative Modelling of Cleaning and Decontamination

Engineering and Physical Sciences Research Council

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Figure 2 and Table 4 updated 12 April 2022

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Executive Summary

Cleaning and decontamination operations are practised daily, worldwide, consuming large amounts of time, energy and other resources – particularly water. They underpin the safe and effective operation of hospitals (e.g. COVID-19, MRSA), industry and the home, and are important to 7 UK Government Departments and 18 Agencies as well as 12 broad sectors of UK industry and everyday life.

At present the design and development of cleaning and decontamination methods is largely empirical and not suited to meet the grand challenges associated with sustainability, healthcare, smart manufacturing and the management of responses to new hazards.

Cleaning and decontamination operations are highly multidisciplinary, linking the physical, chemical, biological and health sciences to fluid and device mechanics, data management, and risk. Quantitative modelling provides the essential framework for linking these.

An EPSRC-funded workshop was held in April 2021 to identify the needs and challenges involved in quantitative modelling of cleaning and decontamination and to develop a roadmap for future activity, which will build on the existing world-leading UK expertise in this area. Needs and challenges exist in the areas of sustainability, risk, diversity, networking, training, sensors and underpinning sciences. The Roadmap identifies out a framework to tackle these through strategic investment in communication, community, training and particular aspects of the science base.

The state of the art in quantitative modelling of cleaning and decontamination is outlined here along with the Roadmap.

A web portal has been established at www.modcad.org to provide an access point for resources and networking.

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Introduction and Context

Cleaning is the removal of unwanted material from a surface, an object or a fluid, and is a universal activity, practiced worldwide in the home, in industry, in the built and the natural environment. Decontamination involves removal down to the organism or molecular level and represents a rigorous and intensive level of cleaning. Cleaning can relate to unwanted species on a surface (including solid walls, flexible sheets, skin, porous and non-porous materials) and in a bulk fluid.

Cleaning is performed to allow the material or unit with the affected surface to be used again (restoring operation), used for a different product or service (avoiding cross-contamination), to be sold, or to function safely.

The regularity and number of cleaning operations performed daily means that it consumes large amounts of resources, both in terms of staff and operating time, energy, chemicals and water, and affects the financial and environmental sustainability of many human activities.

> *Example*: The costs associated with fouling and cleaning can constitute 80% of the production costs in the dairy industry. Eide *et al.* (2003) reported that up to 30% of the energy consumed in dairy processing is linked to cleaning. Each litre of milk processed requires about 1.8 litres of fresh, clean water. Elsewhere in the food and drink sector, a litre of beer can consume up to 7 litres of fresh water.

Cleaning also generates waste streams and for some applications involving hazardous materials the waste streams are also hazardous: cleaning then involves relocation of the material in a safe and controlled fashion. The environmental impact of cleaning wastes can be a significant factor in the selection and management of the cleaning operation, and a matter of growing concern to authorities and the general population.

> *Example:* Dairies typically use solutions of sodium hydroxide to remove protein deposits. These are strongly alkaline (pH > 11) and the spent solution needs to be neutralized before disposal. Even then, the amount of sodium discharged in waste streams can be problematic.

Cleaning impacts people, places and production processes. Cleaning operations can be strongly localized, as in factories, or widespread and unevenly distributed when related to populations (*e.g*. hospitals, urban environments).



Table 1 lists *some* of the sectors in the UK where cleaning and decontamination play a critical role in everyday operation, and the associated scientific challenges.

Table 1 Examples of major UK sectors with intensive cleaning activity (in alphabetical order)

Sectors	*Examples of critical cleaning operations*	*Scientific challenges*
Agriculture	Decontaminating animal houses; combatting disease, *e.g.* wilt, avian flu; cleaning product for market	Distribution of cleaning agents; accessing infected areas; minimal processing
Energy	Gas scrubbing, pollutant removal; solar panel, wind turbine cleaning	CO_2 removal; fine particulates; cleaning in arid regions
Environment	Groundwater contamination, oil spills, aquifer contamination, air pollution, pollution in rivers, lakes and oceans, space debris	Multiphase flow in porous media; washout, large volumes
Food and Drink	Product changeover; removing fouling deposits; avoiding cross-contamination	Variability in products, complex rheologies and biologies
Healthcare/public health	Cleaning to deactivate/neutralize or remove pathogens from surfaces	Large areas, wide range of contaminants; complex surfaces
Hospitality	Laundry, kitchens, rooms	Complex soils
Military/public health	Decontamination of surfaces contacted with toxic agents	Identifying best cleaning method; limited resources; hazardous substances; complex environment
Nuclear	Decommissioning of reactors and fuel processing units	Hazardous materials, complex environment - strict inventory control, and waste compatibility challenges.
Personal care products	Switch-over between products	Complex fluids - don't flow easily
Pharmaceuticals	Avoiding cross-contamination between products and batches	Complex chemistries - ensuring validation
Shipping	Hull cleaning to reduce drag	Non-toxic adhesion reduction; in situ removal
Water	Clearing blocked supply lines	Complex biofilms, hygiene

The level of cleaning required, essentially the answer to the question 'How clean is clean?' varies noticeably between applications. The differences in the target or critical cleaning attributes create challenges when transferring results from one sector to another. The **length scales** involved are illustrated in Table 2.

Table 2 - Levels of cleanliness

Length scale	*Cleanliness criterion*	*Detection method*
m-km	Room/area free of contaminants	Sparse sampling, mobile sensors
mm-m	Process performance restored	Operating data, visual, on-line sensors
10s of microns	No visible biofilms Residual coatings removed	Visual, staining in situ, on-line sensors, Coupons (tested in-situ and ex-situ)
5-10 microns	Bacterial cells removed	Swabbing (tested ex-situ) Staining + visualization in situ
1 micron	No spores	Swabbing
Sub-micron	Optically clean	Coupons (tested ex-situ)
Nanometre	Chemically clean	-

The timescale required to achieve cleaning depends both on the nature of the soil and the level of cleaning required, which vary widely between sectors. In some sectors cleaning operations determine the operating schedule (*e.g.* health and personal care) whilst in others the delivery of resources to perform cleaning is the rate-limiting step (*e.g*. toxin release response, cleaning in arid environments).

In practice, cleaning and decontamination operations involve three stages for a known soil:

(1) Cleaning method selection, design and development;

(2) Identification of a validation method;

(3) Monitoring performance and data management

Protocols for identifying the components of each stage are covered by guidelines and codes in some sectors, whilst in others the methods employed are strongly empirical and based on tradition.

The traditional method for selecting and optimising a cleaning method is often presented using the construction known as Sinner's Circle (Figure 1(a)), which represents how the different agents can be combined to achieve a desired level of cleaning.

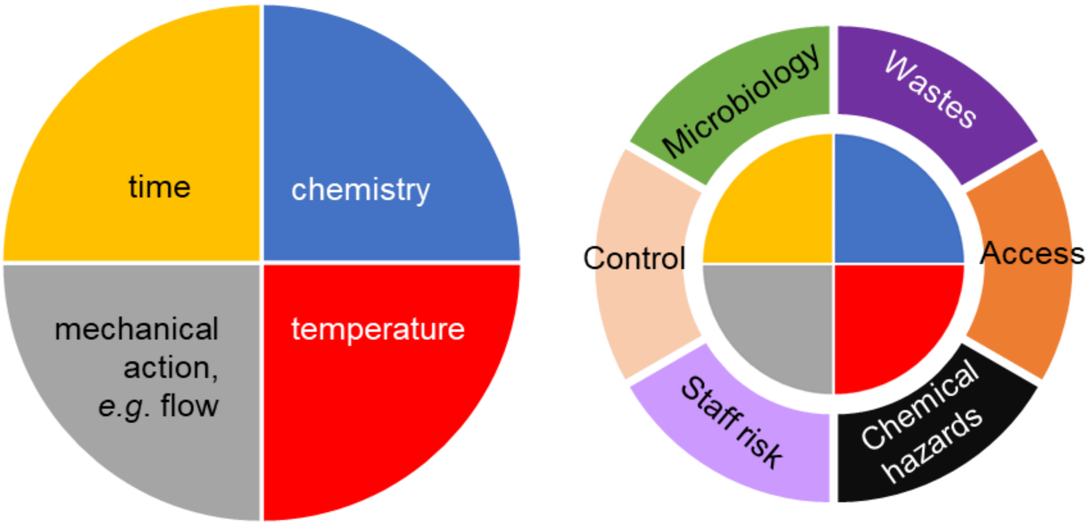


Figure 1 Schematics of cleaning: (a) detailed interactions (Sinner's Circle) determining cleaning mechanisms and performance; (b) overall considerations for implementation.

Modern cleaning applications, however, need to consider the impact of a cleaning on several systems, as illustrated in Figure 1(b). In applications such as healthcare and emergency responses, cleaning is one system within a matrix of systems and this brings with it challenges of complexity, data management and timely decision making.

Motivation

A significant amount of UK resources is devoted to cleaning and decontamination operations. The cost of cleaning and decontamination is rarely quantified as the expenditure is often lumped within general operating and maintenance costs.

The UK Cleaning Products Industry Association reported sales of **£4.5 billion** in 2021, directly employing **10,000 people**, many in small and medium enterprises. Global cleaning product manufacturers such as Diversey reported sales of approximately $2.6 billion in 2017.

The UK Nuclear Decommissioning Authority estimated the cost of decommissioning civil nuclear sites at **£132 billion** over 120 years in 2020.

In addition to risks to human and animal health, the cost of incomplete cleaning or decontamination in the food, healthcare, water and hospitality sectors is high, in terms of legal settlement, product recalls, lost markets and reputational damage. The Food Standards Agency estimates that there are **2.4 million** cases of foodborne illness per year in the UK, whilst estimates produced by the World Health Organisation indicate foodborne diarrhoeal diseases cause 550 million cases and 230 000 deaths worldwide a year.

The Salisbury Novichok clean-up has yet to be costed, but Table 3 overleaf indicates the resources involved.

Table 3 - Resources reported for the Novichok clean-up in Salisbury

	7000+ samples analysed
	190 military personnel plus contractors and Dstl staff
	12,800+ hours spent in personal protective equipment (PPE)
	28 shipping containers of contaminated waste collected
	540 m^3 waste sent for incineration

The importance of foodbourne illness is growing because more serious cases are treated with antibiotics. While almost ten million people die from cancer every year, the UN Ad hoc Interagency Coordinating Group on Antimicrobial Resistance has stated that drug-resistant diseases could cause 10 million deaths each year by 2050 (equalling those from cancers) and damage to the economy as catastrophic as the 2008-2009 global financial crisis. By 2030, antimicrobial resistance could force up to 24 million people into extreme poverty.

Currently there have been 5.5M deaths worldwide due to COVID. Antimicrobial resistance and the impact of deadly pathogens can be slowed and reduced by suitable, effective cleaning and disinfection measures.

Need

The need to improve the selection, performance and deployment of cleaning and decontamination operations, based on scientific understanding, stems from

(a) The importance of maintaining hygiene standards in public and working spaces; this has become significantly more important through the COVID-19 pandemic and will be important as the world recovers;

(b) The resource consumption, environmental impact and carbon footprint of cleaning activities and the supply chains required to support these operations;

(c) The need to improve the performance of key industrial sectors (food, pharma, fast moving consumer goods (FMCG), nuclear);

(d) The need to be able to respond to new challenges, *e.g.* the 2018 Novichok poisoning, COVID-19, cleaning of microfluidic devices and distributed manufacturing units.

These have all been identified as UK Government priority areas, via EPSRC programmes in Defence, Energy, Food, Health, Manufacturing the Future, Net Zero Strategy and Sustainability. These topics are important to Government Departments and Agencies such as DEFRA, Environment Agency, Health, Met Office and MoD. They also represent areas where the UK assists other countries via overseas aid and development.

Table 4 illustrates the range and breadth of activities, using England as an example. Similar structures exist in Scotland, Wales and Northern Ireland. The role of Departments varies from inspection, approving contractors to conduct cleaning operations, providing frameworks for local authorities/businesses, sponsoring research and advising Government on standards and regulations.

Many of the mechanical actions involved in cleaning and decontamination rely on fluid flows. The UK has internationally leading fluid mechanics activities, detailed in *Our Fluid Nation*, published by the UK Fluids Network in September 2021. Fluid mechanics underpins £13.9 billion pa UK industry, employing more than 45,000 people in 2,200 companies. Cleaning and decontamination activities were highlighted in the Productivity and Resilience portfolio.

Within Europe, the importance of producing surfaces to reduce fouling and hence the amount of cleaning is evidenced by recent RIA calls including Horizon-CL4-2021-resilience 01-20: Antimicrobial, antiviral, and antifungal nanocoatings and Horizon-CL4-2022-twin-transition-01-02: *Products with complex functional surfaces*.

This Roadmap was generated as part of EPSRC Workshop Grant EP/T033991/1. A 3 day international virtual meeting was held in April 2021 at which experts in the field identified the state of the art, needs and challenges in the area. A summary of the meeting, including the presentations, is available at www.modcad.org.

The Roadmap was discussed at a hybrid follow-up meeting on 20 September 2021.

Figure 2 summarises the range of applications involved and the shared issues: it is difficult to identify a topic where cleaning and decontamination are *not* important.

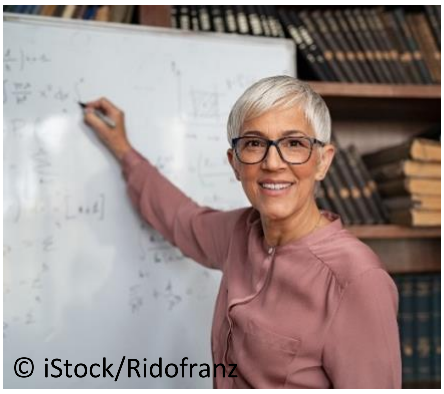
Table 4 - Government Departments and Agencies in England with cleaning interests.

		Environment				Large scale infrastructure			Businesses			Other		
Departments	Agencies and public bodies	Pollution of land or water	Oil spills	CBRN contamination	Air pollution	Cleaning roads	Nuclear de-commissioning	Water supply & wastewater treatment	Food & drink industry	Pharma & chemical industries	Farming & abattoirs	Health & social care	Food hygiene at home	Waste
Department for Environment Food & Rural Affairs		■	■	■	■			■			■			■
	Environment Agencies*	■	■	■	■									■
	Natural England	■												
	Water Services Regulation Authority (Ofwat)							■						
	Drinking Water Inspectorate							■						
	Marine Management Organisation		■											
	Animal & Plant Health Agency										■			■
Department of Health & Social Care		■		■	■					■		■		
	UK Health Security Agency	■		■	■									
	Medicines & Healthcare Products Regulatory Agency									■				
	Care Quality Commission											■		
Department for Business, Energy & Industrial Strategy			■	■	■		■							■
	Oil & Gas Authority		■											
	Offshore Petroleum Regulator for Environment & Decommissioning		■											
	Nuclear Decommissioning Authority (inc. Sellafield)			■			■							
Department for Transport			■	■	■	■								■
	Highways England		■	■		■								
	National Highways		■	■		■								
	Maritime & Coastguard Agency		■	■										
Department for Work & Pensions			■	■	■				■	■	■			■
	Health & Safety Executive		■	■	■				■	■	■			■
Food Standards Agency									■				■	
Ministry of Defence		■	■	■			■							
	Atomic Weapons Establishment			■			■							
	Defence Science & Technology Laboratory			■										
The Crown Estate		■	■								■			

*Environment Agencies include SEPA, Natural Resources Wales and NI Environmental Agency.

Figure 2: Schematic highlighting the broad range of sectors where cleaning and decontamination problems are important, and the related challenges

Why quantitative models?



This Roadmap focuses on quantitative models in cleaning and decontamination.

These are numerical and theory-based tools which allow the attributes of a cleaning operation to be predicted or compared, based on scientific principles and knowing the values of associated process and contextual parameters.

These models are essential for

(1) Selection and design of cleaning operations, particularly for new scenarios: *e.g.* determining how much a new scenario will cost and how much better it will work.
(2) Optimisation of existing processes, and adjusting these for different tasks or products.
(3) Transferring the results from one application to another.
(4) Quantifying resource consumption, waste generation and operating costs.
(5) Supporting management decisions involving resource allocation, risk.
(6) Life Cycle Analysis (LCA) and sustainability studies.
(7) Conforming to industry standards, regulations and legislation frameworks.

The level of detail required for each scenario varies, and different types of models are appropriate for different outcomes: risk assessment tools are often statistical in nature, and require different data inputs as well as detailed processing simulations. The models can be classified as *empirical* (correlations based on underlying scientific principles), *phenomenological* (written in terms of basic principles, with adjustable terms) and *simulation* (based on fundamental governing equations).

Length scales

The dimensions involved in cleaning and decontamination are very diverse – in terms of mechanistic detail, ranging from the machine scale to that of an organism or molecule on a surface – while in spatial area ranging from a single tool or container to a hospital or city.

Time scales

Cleaning operations can be very quick: lasting milliseconds with strong cleaning flows (jetting, spraying, high-pressure flow through pipes), or very long, lasting hours when soaking, low reactivity or diffusion times are involved, and up to decades in the case of slow flow through porous media (cleaning of aquifers). These depend on the methods used to clean, as well as the size and type of the region requiring cleaning.

Method

The scientific method involves identifying the dominant mechanistic step(s), establishing the key parameters, framing the mathematical problem, testing and validating the model, calculating the outcomes and using these to establish the most likely behaviour.

Accurate models allow numerical experiments to be performed (*e.g.* on a digital twin) to establish how the real system will behave or the likely effect of a change in an input of the soiling material or the cleaning protocol. They also allow results to be scaled up or scaled down, as changes in mechanisms arising from different length scales can be identified without many experiments. When the unwanted material is hazardous, expensive or not suitable for lab tests, this is key to reduce risks, costs and time.

In theory, a detailed model should be able to be used for related cleaning applications. This is rarely achieved because:

(a) **Core science insight is required to identify the key mechanisms**. Cleaning and decontamination problems are viciously *multidisciplinary*. The unwanted materials are often complex in nature, and non-uniform. Biological materials, for instance, often evolve *in situ*, and the models thus need to be tuned for the system under consideration, whilst some fundamental processes are still poorly understood.

(b) **These are not simple calculations.** The problems are mathematically complex because they are inherently dynamic and the underlying equations are *messy*: there are frequently several key factors involved, each of which influences the outcome in a complex interplay which can be challenging to compute even numerically, and so calculations have to be done for subsets of factors and for a limited number of regimes.

(c) **Soils are rarely well understood.** The values of the parameters involved in the models are often not known accurately enough, or are difficult to measure. Modern scientific instruments are usually designed to work at finer scales, which is suitable for decontamination. However, cleaning of micro- and macro-scale soiling material – which needs to be done before the decontamination stage – involves thicker, often composite layers which need to be studied *in situ* and in *real time*. This can require the cleaning procedure to be adapted in real time too.

(d) **Robust methods are needed.** Models are usually developed under ideal situations, for example considering one reaction in a process under well-defined conditions, whilst in practice conditions are less well defined and material compositions vary.

(e) **Defining 'clean' can be difficult.** The end point of cleaning (*i.e.* when is it clean enough?) may be the most difficult part of the process to predict and is also the most difficult part to validate in practice. Selection of the 'clean' time will depend on the impact of getting it wrong.

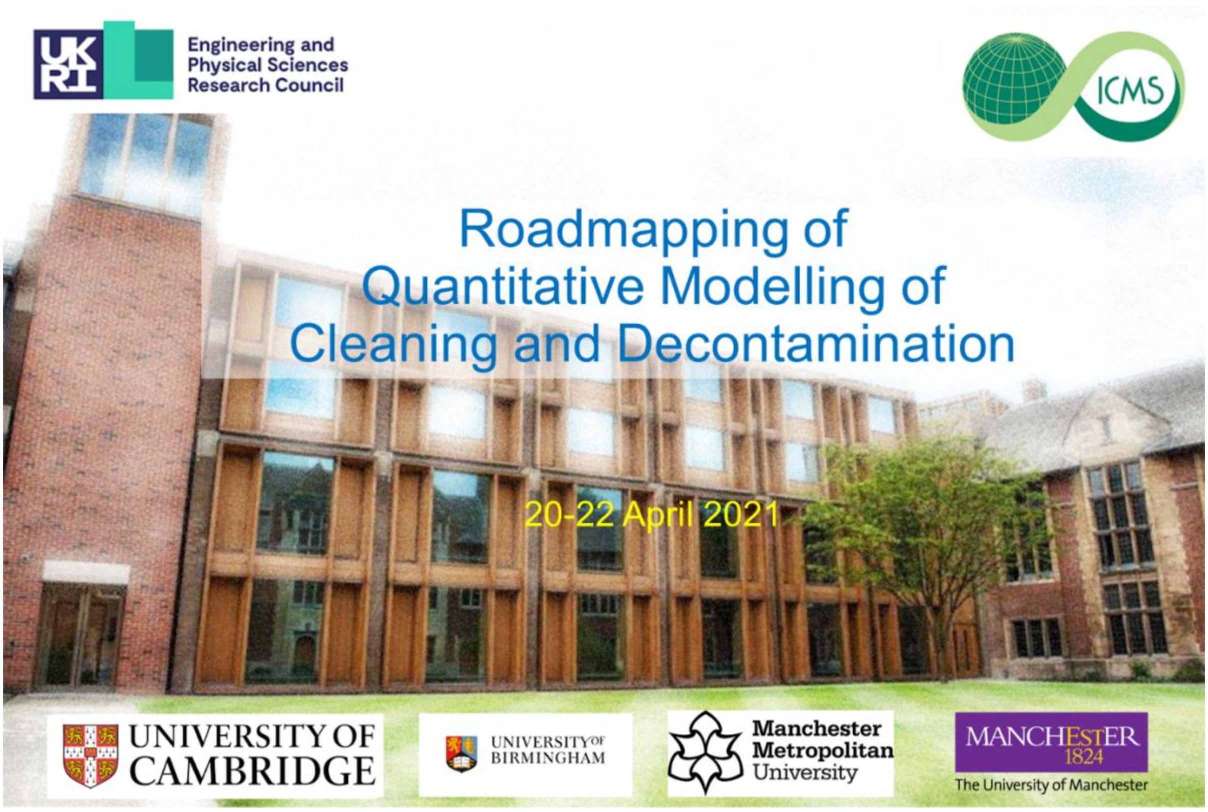
UK capability and track record

The UK has a strong, and in many cases world-leading, research base in the disciplines associated with cleaning and decontamination. These include the physical sciences, particularly chemistry, biological sciences, engineering, public health, environmental science, statistical and applied mathematics.

The core capability in fluid mechanics is detailed in the *Our Fluid Nation* report. Research groups in universities, industry, government departments and agencies are actively pursuing research in cleaning and decontamination, publishing that research, working with end users, organizing conferences and training researchers.

The 2014 Research Excellence Framework (REF) impact studies included 17 cases on cleaning and 7 cases involving decontamination. The *80* participants at the Workshop offer a snapshot of that activity (see Appendix A).

Three of the keynote speakers were deliberately invited from outside the UK to offer international perspective and benchmarking. The UK research community in the field has widespread links with the global research community. These were strengthened at the meeting, with participants joining from 12 different countries.



Needs and Challenges

The following headline needs (N) and associated challenges (C) were identified.

N1 Sustainability

Environmental sustainability considerations and prioritization of scarce resources means that the choice of methods and chemicals that can be used in cleaning will narrow in future. Clever cleaning technologies and better use of existing resources, including the recycling of cleaning agents, need to be developed now.

Going forward, more systems and devices will need to be designed to be cleaned, rather than retrofitted for cleaning.

N2 How Clean? = Risk

The question of 'How clean is clean' arises in all cleaning and decontamination operations. The critical cleaning attribute(s) have to be based on assessments of impact and acceptable response, rather than simply the ability to detect the material. This is an important point since residual material on a surface may be transferred into a clean product. Complications arise in biological contexts since the detection of a material does not validate its potential impact. For example, although DNA or protein may be detected on a surface, this is not necessarily indicative of the presence of a viable pathogen or an allergen. As technology changes detectability limits, systematic ways of processing the data and deciding performance based on measurement patterns, cleaning efficacy and sensible detection criteria are needed. This requires understanding of the consequences of different levels of performance, together with quantitative **risk** analysis, training and communication of the results to all stakeholders.

C2 Communication

The calculation of risk and its consequences, and the communication of the findings in appropriate ways is important for developing trust between all stakeholders. The COVID-19 pandemic has highlighted this challenge in the age of social media. These topics are not currently taught in many scientific programmes, and requires input from behavioural scientists to identify suitable strategies and tools to equip workers to change the narrative in these areas.

N3 Diversity

The topic is highly multidisciplinary. There is a strong need to establish and communicate/exchange what has already been done in other fields, in order to avoid duplication, and to support advances in new fields by building on existing effort.

This needs to be systematic, so it can be built on and developed. An inclusive framework which connects existing researchers, experts, facilities and new users needs to be developed. This is helped by the fact that cleaning and decontamination activities are often pre-competitive for most industrial sectors, so participants are often able to share information without compromising commercial confidentiality. In some sectors this is hindered by cleaning not being pre-competitive for companies performing cleaning or selling cleaning products, where there is a commercial need to protect know-how.

C3A Language

As in all interdisciplinary activities, there are issues with communication and language. A common taxonomy needs to be developed to allow researchers and users to share information and concepts efficiently. There are parallel challenges in developing the language for communication between researchers/users and public bodies, regulatory bodies, and the general public.

C3B Mindset

In cases where cleaning and decontamination questions in one sector can be addressed by adapting results from another, the complexity of the underlying problem can require considerable effort without immediate economic return. For instance, measurement of a key parameter may need to be done for the first time.

In the current UK funding environment, resources to support suitably expert researchers to work on topics which are not viewed as fundamental research yet deliver core capability in this sector can be difficult to secure, as is funding for academic work in the field to cross the 'implementation gap' into commercial practice. Although multidisciplinary and applied projects are encouraged, they require a different skill set, and as such grant proposals in this area can often be criticized when assessed by reviewers without the applied or multidisciplinary expertise.

N4 Network

In technology transfer and translating results from one field to another, it is important to understand the key drivers and constraints in each application, and the critical cleaning attributes. This will often require input data which may not be known accurately. Establishing a network of researchers who are able to make such measurements, or access reports containing such information, is required.

C4 Profile

Cleaning and decontamination is a multidisciplinary activity without an academic 'home' in the UK, partly as a result of it not attracting research council attention. Development of an effective network would require strategic input, supporting activities for an extended initial period, in order to establish a network that could be self-sustaining in the longer term. Indeed, cleaning and decontamination are neither superfluous nor trendy activities: they are essential to human wellbeing, even more so in the complex, dense and strongly interconnected world of today and tomorrow.

It should be remembered that ineffective cleaning can lead to multiple cases of disease, and in some cases even death, especially where bacterial contaminants are of concern *e.g*. contamination of food products by *Escherichia coli* 0157:H7 or *Listeria monocytogenes*.

N5 Training

Training and developing researchers, users and other stakeholders with the necessary knowledge of the relevant disciplines is essential to develop UK capability in these areas. At present there is *no* structured provision of training within undergraduate courses or specialised Masters degree programmes. Research students glean knowledge related to their topic as part of their studies, but rarely have an opportunity to receive a structured description of the field or an opportunity to present their results to a mixed, knowledgeable audience.

There are exceptions in certain sectors (*e.g*. food processing, pharmaceutical manufacturing), and it was noted by those participating in the UK Fluids Network Special Interest Group on the Fluid Mechanics of Cleaning and Decontamination that this activity strongly enhanced the development of young researchers. A coherent training package would cover aspects of key science, mathematical concepts (but not expertise), life cycle analysis, risk management and communication. A programme that is strongly linked to industry would be forward facing and would provide a novel and valuable resource to business, by incubating multidisciplinary research to tackle key issues.

C5 Image

The topics of cleaning and decontamination are not 'sexy' and have not to date attracted talent or research council attention. This is partly due to familiarity with the topics in the domestic sense and the low status/value in many commercial settings (with some exceptions): cleaning can be seen as a necessary but mundane or annoying chore, taking time and resources away from primary tasks. Historically it has not been viewed as a priority but this is changing owing to the growing importance of environmental and sustainability targets.

The 2018 Salisbury Novichok episode, the development and transmission of antimicrobial-resistant bacteria and the COVID-19 pandemic have demonstrated how new thinking is needed in order to develop the fundamental understanding of these fields and implement effective new methods quickly. The technical content of the Workshop showed that cleaning and decontamination is underpinned by state-of-the-art fundamental scientific understanding, and their implementation requires cutting-edge technologies. Cleaning and decontamination must now be taken seriously and given priority in such a changing world.

N6 Sensors

Many cleaning operations rely on old measurement methods and sensor technologies. There is a widespread need to develop **sensor** techniques which are versatile, reliable, scaleable and which eliminate the variability inherent in human testing. Both portable sensors as well as in-line sensors for aseptic processes are required. This is challenging as the sensor data needs to represent the region around it faithfully rather than the conditions local to the sensor. This is a field with opportunities for machine learning, artificial intelligence and uncertainty quantification in data interrogation and data fusion.

There is a similar need for instrumentation which can make measurements *in situ,* in real time and under realistic conditions, for studying soil layers or deposits which cannot be transferred to standard laboratory devices. This will generate new types of data, the interpretation of which fits under N4.

N7 Underpinning Science

Fluid mechanics is the science underpinning many cleaning operations. The detailed mathematical models describing cleaning are complex, featuring dynamic problems, multiphase flows, complex fluids and interfacial phenomena such as moving contact lines and surfactant effects. These give rise to fundamental research problems with links to other fields (*e.g.* microfluidics, flow in porous media, rheology) and a need to develop the mathematical methods for these problems at the length scales and timescales which arise in cleaning.

C6 Complexity and Capacity

The numerical simulation of cleaning scenarios based on the mathematical modelling of fundamental physical, chemical and biological processes can be also very challenging, even for modern computers. This is due to the wide disparity of length and time scales associated with cleaning scenarios, which require high resolution simulations that can take substantial computational resources. The number of factors involved can be large and the geometries complex, again necessitating a large number of simulations in order to sample a representative number of scenarios. In some cases the complexity can be reduced by mathematical methods. Once constructed, the models can be used in numerical experiments to map out regions and to identify simpler models that give acceptable accuracy for end-users and management tools.

Testing of the mathematical models at laboratory and pilot scale in order to ensure appropriate scale up are essential, and the data from these physical tests need to be fed back into the simulations to develop both the mathematical models and the efficacy of the cleaning systems. Currently, there is no such process for this. In the food sector, New Zealand leads the way with specialized facilities to carry out such routine testing. In order for the UK to compete and to be prepared, we must expand our facilities now, rather than approaching such issues after an event.

Vision for the future

The April workshop highlighted the commonality of many topics in cleaning and decontamination across different sectors, as well as the currently strong level of research in these sectors in the UK. Since cleaning and decontamination often fit within a pre-competitive space there is much scope for collaborative research and learning, thereby making best use of available resources.

Researchers in the field need to combine *depth* – answering specific questions - and *breadth* – ensuring that their findings fit within the wider context and translation – providing industry, the medical profession and other businesses with meaningful data. This can be supported UK-wide by

(1) A database of published and ongoing research in cleaning and decontamination, structured to enable translation of research from one field to another;

(2) A community linking researchers and users in the area, supporting interdisciplinary exchange and knowledge transfer;

(3) Training materials covering areas such as risk management, life cycle analysis, validation *etc.* for those conducting research in the field, to provide contextual tools to accompany the research tools that they will develop in the course of their research;

(4) Materials to help the general public and decision makers in industry and government understand the concepts involved;

(5) Strategic allocation of resources for funding research in this area, to strengthen the existing research base and ensure its longevity by attracting new researchers into the related fields.

How to get there – the Roadmap

There has been an unprecedented level of activity related to hygiene and cleaning as a result of the COVID-19 pandemic. This offers an opportunity to change the narrative in the public and academic eyes about the value of research in this area. It also provides an opportunity to establish a world-leading nation-wide network linking research in these fields, as well as attracting and retaining talented researchers.

The Roadmap (Figure 3) shows four strands of activity for the period 2022-2030, assuming that a Doctoral Training Centre could start in 2023.

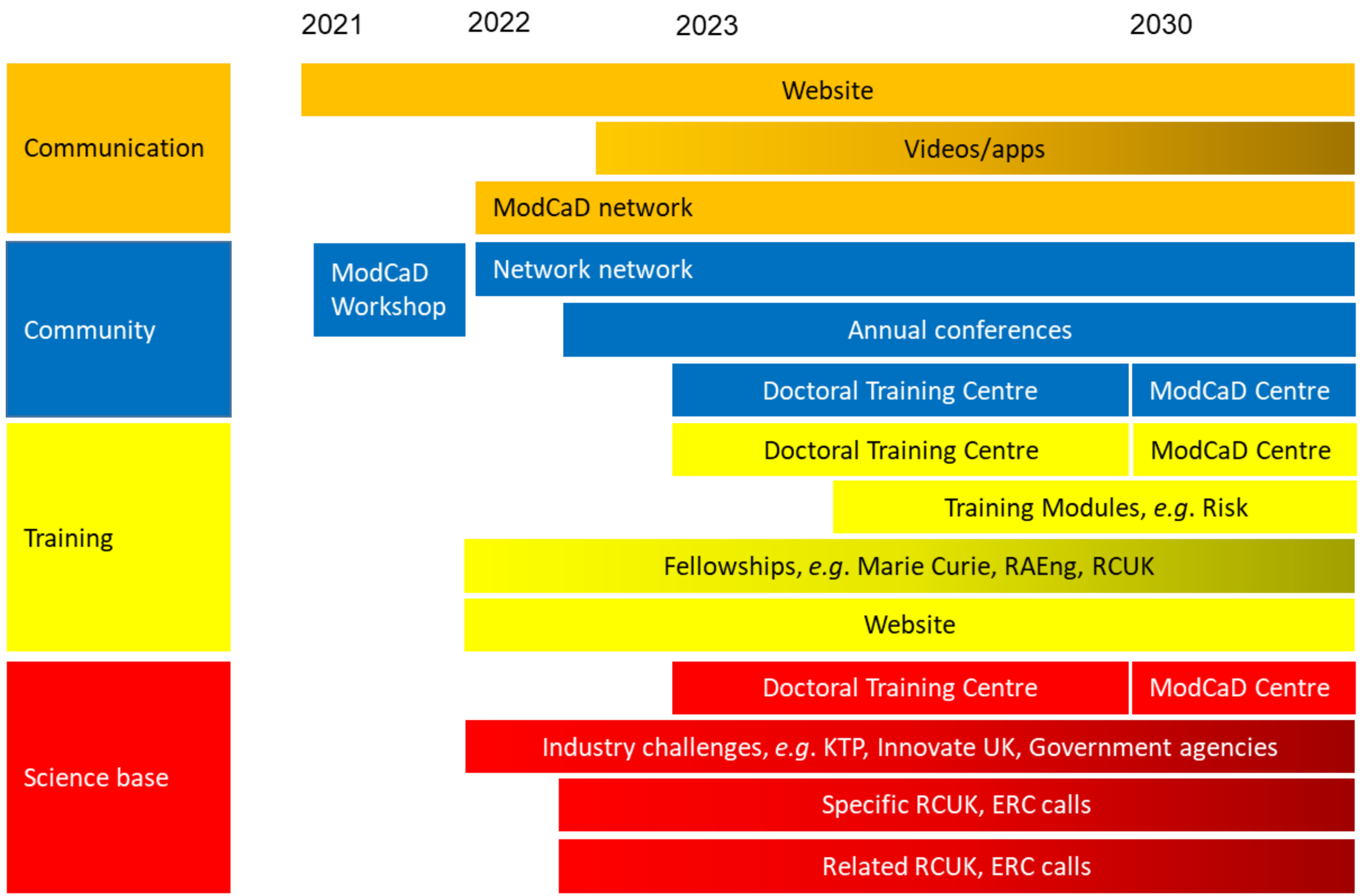
RM1. Communication – linking those active in the area to each other and to the wider population of users, researchers, and interested groups.

> Workshop Grant EP/T033991/1 has generated a legacy website containing an annotated database of research related to cleaning and decontamination and for the first time brought workers from many different areas together to discuss their individual and similar cleaning and decontamination needs. The website will provide a gateway to a network of researchers and users active in cleaning and decontamination. Videos, apps and other learning materials generated by the community will be hosted and linked to the website.

RM2 Community – activities which bring those working in the field together on a regular basis for updates, learning about challenges, debate and discussion.

> A ModCad network group has been established on the Linked-In platform based on those who attended the April Workshop has been established. Its longer-term maintenance, development and support need to be underwritten.
>
> The UK Fluids Network activity saw real benefit from regular meetings, bringing 221 people together over the 3 years of the C&D SIG. This will be continued in the form of an annual meeting, initially connected to an existing UK-wide conference.
>
> The Community, Training and Science Base strands are best integrated by the establishment of a **Doctoral Training Centre (DTC) in Cleaning and Decontamination**. Operating under a hub and spoke model, the DTC will automatically support the development of the community. A DTC will also establish the strategic importance of the work in academic circles and facilitate colleagues in different disciplines and centres to work together. Equal value will be given to activities which transfer results from one sphere to another, and those which work on fundamental understanding. **The community required to support the DTC already exists**. The cost of a Doctoral Training Centre (typically £8M over 5 years) is a fraction of the cost of a major cleaning and decontamination incident.
>
> The success of the DTC will lead to the establishment of a RCUK/industry/government funded centre which is labelled the **ModCaD Centre** on the roadmap. This could include dedicated facilities, depending on the resources available and partnerships involved.

Figure 3 Roadmap for Cleaning and Decontamination



RM3 Training – covering a wide range of resources and activities relevant to those working in the area. In addition to the materials and data base on the website, this will include:

DTC training of PhD-level researchers with a wider understanding of topics in cleaning and decontamination combined with particular scientific expertise. This will require development of specific training modules which will be made available to the wider community via web-based learning techniques. The practice in other DTCs whereby partners are asked to provide case studies and short-term projects for groups of students to work on as part of their training will be adopted. This is expected to be well-suited for some cleaning and decontamination problems, particularly where those involving translation of methods from one field to another.

The DTC partnerships will be attractive to applicants for postdoctoral research fellowship schemes, as the connections will allow these individuals to develop expertise at different centres seamlessly. This is important in supporting early researchers make the transition into longer-term research and academic positions, ensuring that their expertise is retained. Given the complexity of this area of research, the retention of such expertise is essential. The ModCaD Centre would build on these partnerships and the training framework.

All activities (mini-projects and longer term projects) will have to create a public-facing report/podcast and an app or web-tool that would allow other users or readers to make use of their results.

The annual conference would be integrated into the DTC programme.

RM4 Science base - there are gaps in the fundamental science and understanding, requiring research and development activities at different levels of complexity and timescale. This document has highlighted Needs and Challenges in 7 broadly defined areas.

The DTC will support a range of projects investigating different topics at the PhD level across the spectrum of sciences and mathematics. The ModCaD community will provide a network for hosting other activities, such as shorter term Innovate UK projects, Impact demonstrations and KTP technology transfer work. The DTC will generate skilled researchers able to work on such projects with modest start-up time.

Coherent research programmes for RCUK/Government funding are required in the areas of

- Sensors and instrumentation
- Surfactants, spreading and interfacial dynamics in cleaning applications
- Data management, risk and uncertainty quantification
- Biofilm detection and control – a future without swabbing
- Surfaces for repeated cleaning and decontamination

Concluding Remarks

The Workshop demonstrated that cleaning and decontamination activities are common to a very broad range of applications across the UK, from industry and government to many daily activities. It has also highlighted that the fundamental science behind many of these activities share similarities: it is highly multi-disciplinary, involves many parameters and geometries, and ranges across several length and time scales.

At the moment, cleaning and decontamination processes are often tackled using solutions developed historically for specific industrial problems, without much knowledge of practices elsewhere and, in some cases, the underlying science.

A high degree of know-how and technical knowledge exist, but they are often applied narrowly, to specific problems. Within the academic communities, expertise in specific subject areas can be very deep, but this can make it difficult for non-experts to access and impossible to translate across sectors. There is nevertheless recognition that the multi-disciplinary nature of the science behind cleaning and decontamination requires more communication and exchange across disciplines, as well as engaging with industrial and government stakeholders to translate the fundamental knowledge into practical solutions. Experts with suitable translation skills are needed to lead the way in these activities.

The actions and recommendations set out the steps needed to tap into the current expertise across scientific disciplines, public agencies and industrial sectors, in order to approach problems with a comprehensive and appropriately multidisciplinary view. They promote horizontal communication and exchange between stakeholders and experts to enable them to develop, test and implement quantitative models that can support better solutions to practical problems. This vision also identifies the challenges associated with communicating scientific concepts alongside risk to public or personal wellbeing: current and future generations of experts need to be equipped with training spanning both fundamental and practical aspects.

Cleaning and decontamination issues are not only central to most human activities, they are also critical to the maintenance and growth of a sustainable, healthy and thriving society. To be effective these activities need sufficient funding and time to deliver on their long-term objectives. The price to pay now is small compared to the cleaning and decontamination costs that large scale and complex issues require, whether related to a pandemic, poison threats, large scale pollution events or long-term nuclear decommissioning.

Some profound changes are needed in the way we view and approach cleaning and decontamination problems, but they will ensure that the UK is prepared and equipped to tackle new and existing ones sustainably in future.

Appendix Participants at the April Workshop and/or September Roadmapping meeting

Country of non-UK based participants indicated

Colour coding: Government, Industry, Research/Academic, Young Researcher

Name	*Affilation*	*Discipline/Sector*
Hosam Aleem	University of Manchester	Chemical Engineering
Graham Anderson	Beko R&D	Home appliances
Panagiota Angeli	University College London	Chemical Engineering
Dragana Arlov	Tetra Pak, Sweden	Food Process Equipment
Les Baillie	Cardiff University School of Pharmacy	Pharmacy
Alan Beswick	HSE	Government Agency
Uwe Beuscher	WL Gore & Associates, USA	Cleaning and Filtration
Pete Birkin	University of Southampton	Chemistry
Chris Breward	University of Oxford	Mathematics
Emily Butler	University of Manchester	Mathematics
Sara Casey	Defra	Government
Loïc Chagot	University College London	Chemical Engineering
Melissa Chee	University of Cambridge	Chemical Engineering
Graham Christie*	University of Cambridge	Microbiology
Stuart Clarke	University of Cambridge	Chemistry
Simon Coldrick	HSE	Government Agency
Conor Collins	GSK, Ireland	Pharmaceuticals
Sam Collins	Public Health England	Government
Francesco Conto	University of Cambridge	Mathematics
Mohit Dalwadi	University of Oxford	Mathematics
Stuart Dalziel	University of Cambridge	Mathematics
Antonio D'Ammaro	Beko plc	Home appliances
Kartik Deshmukh	University of Cambridge	Chemical Engineering
Eze Emekwuru	Coventry University	Manufacturing Engineering
Merlin Etzold	University of Cambridge	Mathematics
David Fernandez Rivas	University of Twente/BuBclean, Netherlands	Chemistry
George Fortune	University of Cambridge	Mathematics
Peter Fryer*	University of Birmingham	Chemical Engineering
Geoff Gibson	Pfizer	Pharmaceuticals
Christian Golla	Institute of Fluid Mechanics, TU Dresden, Germany	Physics
Anders Goransson	Tetra Pak, Sweden	Food Process Equipment
Norman Govan	DSTL	Government Agency
Laura Guardi	AstraZeneca	Pharmaceuticals
Cameron Hall	University of Bristol	Mathematics
Ian Hall*	University of Manchester	Mathematics

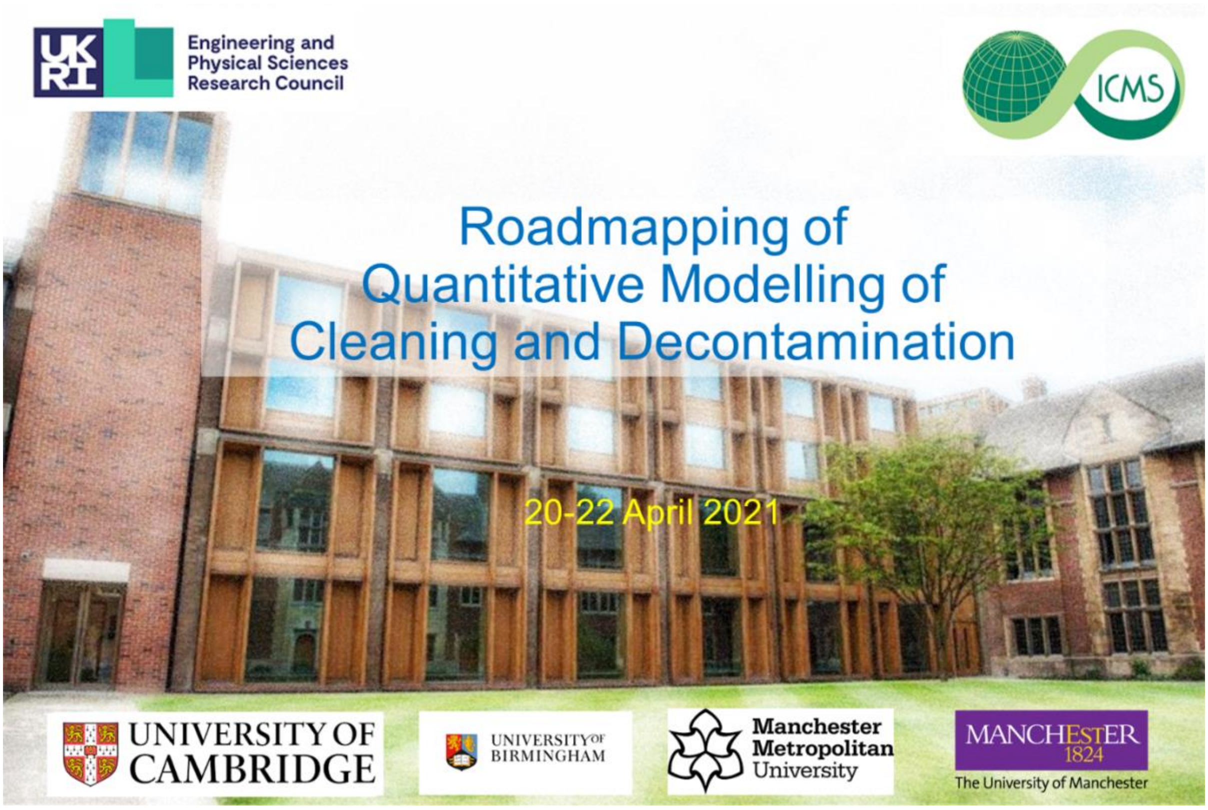
Tobias Hanisch	Fraunhofer IVV, Processing Technology, Dresden, Germany	Mechanical Engineering
Hossein Hassanzadeh	Laval University, Canada	Chemical Engineering
Sarah Hayes	PMTC at University of Limerick, Ireland	Pharmaceuticals
Denny Heldman	Ohio State University, USA	Food Engineering
Lesley Hetherington	DEFRA	Government
James Hewett	University of Canterbury, New Zealand	Mechanical Engineering
Holly Huellemeier	The Ohio State University, USA	Food Engineering
Tom James	Public Health England	Government
Alex Jenkins	Sellafield	Nuclear
Yin Jialiang	Fraunhofer Institute for Process Engineering and Packaging, Dresden, Germany	Mechanical Engineering
Matthias Joppa	Fraunhofer Institute for Process Engineering and Packaging, Dresden, Germany	Mechanical Engineering
Sepideh Khodaparast	University of Leeds	Mechanical Engineering
Kris Kiradjiev	University of Oxford	Mathematics
Dawn Knapek	Procter & Gamble, USA	Home and personal care
Yusuf Koc	Arcelik A.S., Turkey	Domestic appliances
Hannes Köhler	Technische Universität Dresden, Germany	Mechanical Engineering
Sebastian Kricke	Technische Universität Dresden, Germany	Mechanical Engineering
Halim Kusumaatmaja	Durham University	Physics
Julien Landel*	University of Manchester	Mathematics
Sewon Lee	University of Manchester	Medicine
Ellen Luckins	University of Oxford	Mathematics
Mirco Magnini	University of Nottingham	
Brent Mantooth	US Army DEVCOM Chemical Biological Center, USA	Government Agency
Steve Marriott	DSTL	Government Agency
Haz Matar	University of Hertfordshire	
Omar Matar	Imperial College London	Chemical Engineering
Marc Mauermann	Fraunhofer Institute for Process Engineering and Packaging, Dresden, Germany	Mechanical Engineering
Luis Melo	Faculty of Engineering of University of Porto, Portugal	Chemical Engineering
Rakesh Mishra	University of Huddersfield	Mechanical Engineering
Rabah Mouras	PMTC, University of Limerick, Ireland	Pharmaceuticals
Abhinav Naga	Max Planck Institute for Polymer Research, Germany	Physics
Stuart Notman	DSTL	Government Agency
Mathieu Ortega	DEFRA	Government
Lukas Oudejans	U.S. EPA, Office of Research and Development, Center for Environmental Solutions and Emergency Response, USA	Government Agency
Siddharth Patwardhan	University of Sheffield	Chemical Engineering

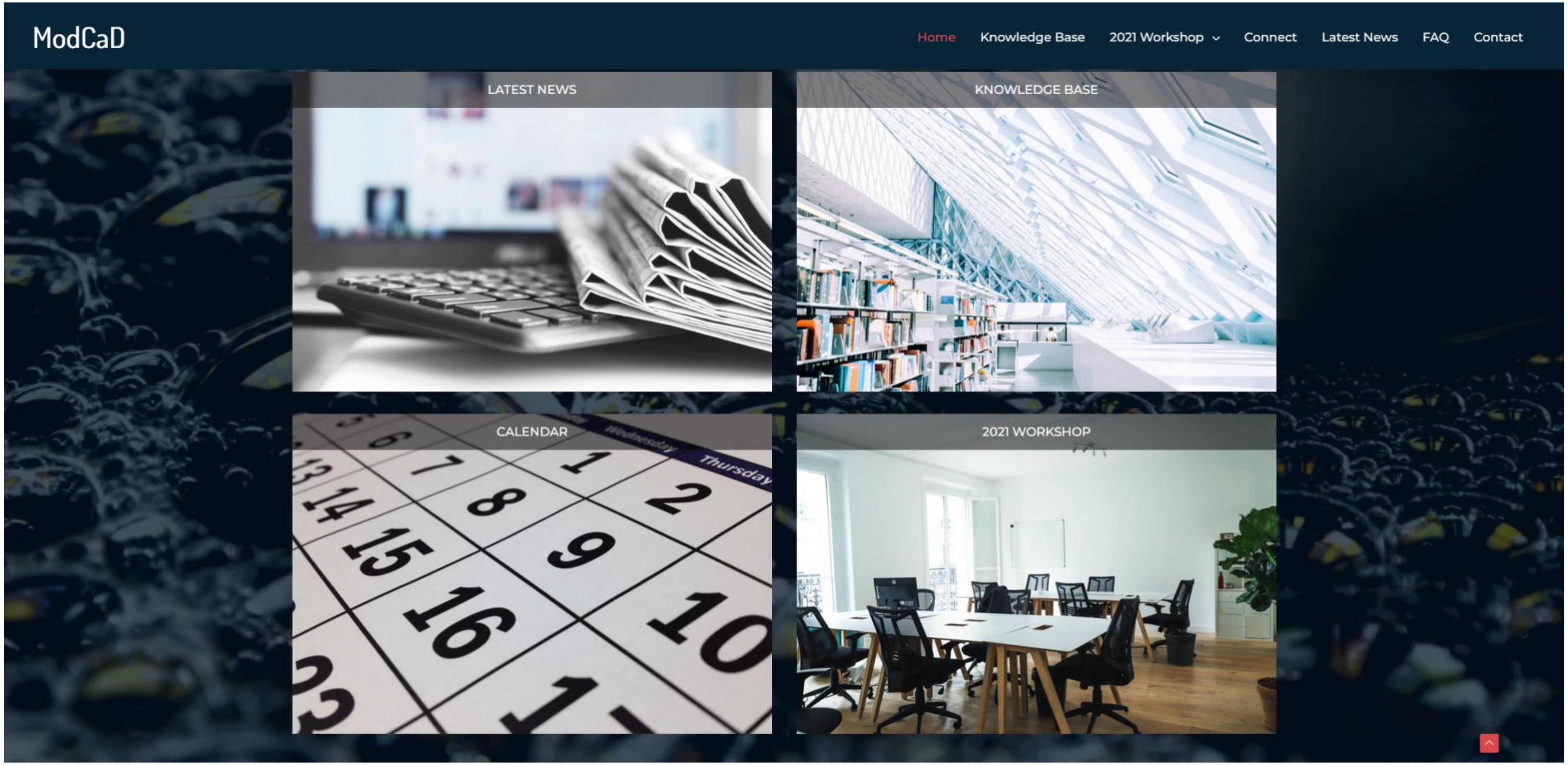
Tom Pearl	U.S. Army DEVCOM Chemical Biological Center, USA	Government
Thomas Pottage	UK Health Security Agency	Government
Rubens Fernandes	University of Cambridge	Chemical Engineering
Parisa Sarmadi	University of British Columbia, Canada	Mechanical Engineering
Martin Seed	University of Manchester	Medicine
Jim Taylour	Chemical Consulting Solutions Ltd	Cleaning consultancy
Allister Theobald	Lubrizol Life Science	Cleaning chemicals
Mark Varady	U.S. Army DEVCOM Chemical Biological Center, USA	Government Agency
Vasu Venkateshwaran	W. L. Gore & Associates, USA	Cleaning and filtration
Nik Watson	University of Nottingham	Chemical Engineering
Kath Whitehead*	Manchester Metropolitan University	Microbiology
Ian Wilson*	University of Cambridge	Chemical Engineering
Worth Calfee	US EPA, USA	Government Agency
Will Zimmerman	University of Sheffield	Chemical Engineering

** indicates Workshop organisers*

Acronyms

DEFRA	UK Department for the Environment, Food and Rural Affairs
DSTL	Defence Science and Technology Laboratory, UK
EPA	Environment Protection Agency, USA
HSE	Health and Safety Executive, UK





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