The Digital Future of Process Chemistry and Technology

Speakers and Programme

18 November 2022, Online and at Burlington House, London

RSC INTEREST GROUP
PROCESS CHEMISTRY AND TECHNOLOGY

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Programme

0900	Registration		For in-person attendees
1000	Introductions	Process Chemistry and Technology Group	An introduction to the topics of the day
1005	King Kuok (Mimi) Hii	ROAR, Imperial College London	The Age of Digital Chemistry
1035	Nicholas Jose	Cambridge University	Applying artificial intelligence to create self-driving chemical laboratories
1100	Stuart Little	JMP Statistical Discovery	Sponsor Presentation: How JMP is enabling the future of process chemistry & technology
1110	Jon-Paul Sherlock	AstraZeneca	Accelerating medicines development through digitalisation
1135	Jason Williams	Research Center Pharmaceutical Engineering GmbH	Incorporating Digitalization and Automation in the Development of Flow Processes for API Synthesis
1200	Panel Discussion	Speakers from the morning session and Andrea Sauerwein, Johnson Matthey	Topics including: What do we mean by "digital" in the context of science, engineering, R&D, and manufacturing? What are the relevant digitalization technologies? How can these technologies enable better process chemistry and technology?
1230	Networking Lunch		Poster exhibition and discussion tables for in-person attendees
1400	Andy Maloney	The Cambridge Crystallographic Data Centre	Late stage ideas from early development: How structural informatics approaches can transform pharmaceutical processes
1430	Joan Cordiner	The University of Sheffield	Digital Future of Chemical Industry - Challenges and Opportunities
1500	Nessa Carson	AstraZeneca	Automate Your Own HTE Workflow
1530	Panel Discussion	Speakers from the afternoon session and Markus Gershater, Synthace	Topics including: What can we learn from examples outside of process chemistry and technology? What skills will process chemists and technologists need for the digital future?
1600	Close for online		Drinks reception for in-person attendees
1730	Close		

King Kuok (Mimi) Hii

LinkedIn

Mimi Hii is a Professor of Catalysis at Imperial College London. She began her independent research career in 1997 with an award of a Ramsay Research Fellowship co-sponsored by an ICI strategic research grant, before she was appointed as a Lecturer in Organic Chemistry at King's College London in the following year. In 2003, she accepted an offer of a Senior Lectureship at the Department of Chemistry at Imperial College London, where she was promoted to a Readership (2009) and Professorship (2016). In 2016, KKH co-led the UK synthetic chemistry community in Phase III of the Dial-a-Molecule Grand Challenge and, in the following year, established UK's first Grand Challenge Institute: the Centre of Rapid Online Analysis of Reactions (ROAR) at Imperial College's new White City Research and Innovation campus. In 2018, she led a successful bid for an EPSRC Centre for Doctoral Training (CDT) in Next Generation Synthesis & Reaction Technology (rEaCt), to champion education and skills training in automation and data-led chemical research. In 2019, she was appointed as an Associate Editor of ACS Sustainable Chemistry & Engineering.

Mimi Hii's research interest in the area of Catalysis is wide-ranging, encompassing molecular design and synthesis, mechanistic and kinetic studies using new analytical tools, and reaction technologies; particularly for performing multiphasic catalytic reactions in continuous flow. To date, her research work has produced >130 scientific papers (culminating in a h-index of 39), 8 patents, as well as a number of monographs and book chapters.

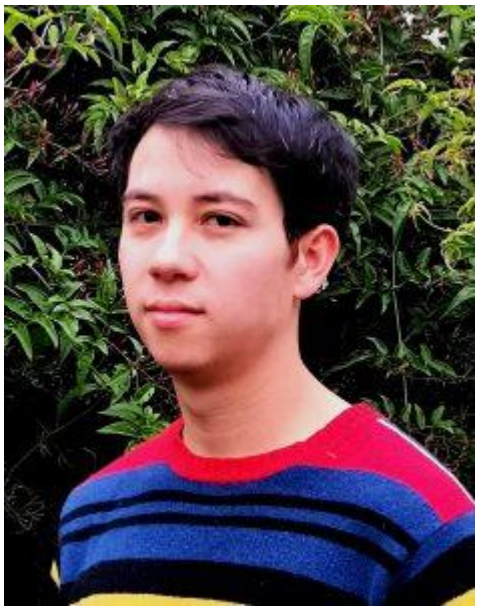
The Age of Digital Chemistry

The 21st Century promises to be the golden age for digital technologies, which in turn, challenges the practice of synthetic chemistry. The vision for 'lab of the future' is the greater integration of automated equipment with data workflows.

In this presentation, I will describe our efforts in inaugurating a centralised automated research facility (ROAR) in the U.K., to support training of early career researchers (rEaCt CDT), as well as supporting technical needs of the synthetic chemistry community. Our attempts to integrate automated data-led processes in our research will be demonstrated with a few case studies, including high-throughput screening in continuous flow and online analytical methods.

Nicholas Jose

LinkedIn



Dr Nicholas Jose is a researcher at the University of Cambridge and Cambridge CARES in Singapore. He is also founder of Accelerated Materials Ltd, a spin-off company that helps businesses create innovative products based on nanomaterials. His research focuses on platform technologies including intensified microreactor technology, novel materials and laboratory automation.

Applying artifical intelligence to create self driving chemical laboratories

Applying artifical intelligence to create self driving chemical laboratories may deliver orders of magnitude enhancements in research productivity. However, implementation of artificial intelligence into realistic use cases often encounters a number of severe hurdles: chemical scientists need to obtain advanced skills in automation/coding, commercial platforms are costly, and suppliers of automated lab devices often "lock" a users into supplier automation workflows. These hurdles limit laboratories across the world from reaching the critical mass required for widespread adoption of "smart" laboratories.

In the pursuit of solving these challenges, and democratising smart laboratories, we have developed FLab,1 an open-source Python coding framework for linking automation, IOT technologies, and artificial intelligence in chemical laboratories. FLab utilises an intuitive, modular, object-oriented architecture to streamline manipulation of shared devices, tasks, AI bots and user interfaces. In this presentation, we describe the inner workings of Flab, and its differentiation from existing frameworks like Labview, ROS and Matlab. We then illustrate its uses in real laboratory experiments, which include a bespoke automated flow chemistry scale-up rig, a high-throughput batch formulation robot, and a system for measuring hydrodynamic parameters in a gas/liquid flow reactor. Finally, we discuss critical aspects for improvement within FLab and within self-driving labs, pointing to new avenues of further research and collaboration in this growing field.

Jon-Paul Sherlock

LinkedIn

Accelerating medicines development through digitalisation

Digital technologies have the potential to significantly accelerate the development of manufacturing processes through virtual experimentation, automation and digital twins. The accelerated delivery of a vaccine in response to the Covid-19 pandemic has redefined the expectations of patients and healthcare systems regarding the speed they should be able to access new medicines. This, coupled with AstraZeneca's strategic ambition of launching 30 new medicines by 2030, mean a genuine transformation in the way medicines are developed is critical. Digital is not just a buzzword, but an opportunity to radically evolve the medicines development process. In AstraZeneca Pharmaceutical Technology and Development an ambitious strategy is being progressed to explore, evaluate and implement different digital solutions. Through this presentation we will share some of the different digital platforms being considered and how what is learnt in development can also influence future manufacturing.

Jason Williams

LinkedIn

Jason Williams is a Principal Scientist at the Research Center Pharmaceutical Engineering (RCPE), based in Graz (Austria). In 2014, he completed an undergraduate degree in Chemistry at the University of Sheffield (UK), with a year industrial experience in medicinal chemistry at AstraZeneca. This was followed by a PhD on the GlaxoSmithKline/University of Strathclyde collaborative PhD Programme, under the supervision of Prof. Billy Kerr. For the majority of this time, Jason was based in the process development labs at GSK Stevenage, working on novel amidation methods enabled by new synthetic technologies, such as flow and photochemistry. Since 2018, Jason has worked in the Kappe group (as part of RCPE), where his research interests are based in the areas of PAT, automation and process control in flow, as well as flow photochemistry.

Incorporating Digitalization and Automation in the Development of Flow Processes for API Synthesis

As the pharmaceutical industry begins to make use of continuous manufacturing technology in synthetic routes toward active pharmaceutical ingredients (APIs), the construction and utilization of automated data-rich systems plays a key role. By combining process analytical technology (PAT) with real-time chemometric processing, vital information on product and impurity concentrations can be obtained. Furthermore, use of supervisory control and data acquisition (SCADA) software allows straightforward automation and data acquisition/exploitation.

Within such a platform, we demonstrate this capability on lab scale for applications including: self-optimizing processes, automated design of experiment (DoE) studies, rapid process model building and model predictive control (MPC). Self-optimization provides an opportunity for coarse process development requiring minimal operator time. Automated DoE can then be used to refine the design space, with a focus on robustness and impurity control. With all of this collected data, process models can be built, for further understanding and use in MPC applications.

By implementing such a workflow during lab scale development, the path toward pilot and manufacturing scale can be thoroughly mapped out and timelines dramatically accelerated. Moreover, this provides an excellent starting point for development of QbD and data-driven control strategies in regulatory submission.

Andy Maloney

LinkedIn

Andy Maloney has a background in chemical and computational crystallography. He joined the Cambridge Crystallographic Data Centre (CCDC) in 2015, where he now leads the Particle Science Team. Working closely with the pharmaceutical industry, his role involves leading research projects in the field of structure-property relationships. His main interest is in Particle Informatics, developing methods to understand the links between crystal structure, particle properties, and downstream manufacturing processes.

Late stage ideas from early development: How structural informatics approaches can transform pharmaceutical processes

Recent advances in digital design methodologies have enabled industrial scientists to move away from time and resource intensive screening techniques to more rapid in silico methods to inform key decisions throughout the pharmaceutical development and manufacturing process. Timely application of such methods can identify potential issues with stability of solid forms or anticipate manufacturing bottlenecks.

With over 1.2 million entries, the information contained in the Cambridge Structural Database (CSD) can provide insight to the link between crystal structure and the properties that govern downstream behaviour. By utilising this wealth of data, informatics-based approaches can be used to visualise and describe key solid state, particle, and surface properties, and how these affect the stability and manufacturability of a solid form.

This presentation will explore how early application of informatics approaches can provide useful information for understanding downstream behaviour earlier in the development pipeline. When combined with computational approaches and best data management practices, these methods have the potential to transform the way we think about manufacturing processes.

Markus Gershater

LinkedIn

Markus is CSO and co-founder of Synthace and one of the UK's leading visionaries for how we, as a society, can do better biology. Originally establishing Synthace as a synthetic biology company, he was struck with the conviction that so much potential progress is held back by tedious, one-dimensional, error-prone, manual work. Instead, what if we could lift the whole experimental cycle into the cloud and make software and machines carry more of the load? He's been answering this question ever since.

Markus holds a PhD in Plant Biochemistry from Durham University. He was previously a research associate in synthetic biology at University College London and a Biotransformation Scientist at Novacta Biosystems.

Markus will contribute to our panel discussions.

Andrea Saurewein

LinkedIn

A solid-state and solution NMR Spectroscopist with a PhD focused on solid-state NMR method development and over a decade of experience in academic and industrial research using both solid- and solution-state NMR methods. Andrea is now R&D Data Readiness Lead at Johnson Matthey, leading the "culture" team that focuses on empowering JM's scientists to be successful in an ever more digital and automated lab of the future that is guided by the FAIR data principles.

Andrea will contribute to our panel discussions.

Joan Cordiner

LinkedIn

Professor Joan Cordiner FREng, FRSE, FIChemE, FAIChemE, CEng moved to academia in 2020 from a 30+ career in ICI, Astra Zeneca and Syngenta latterly as a Technology Manager and Global Risk Manager for Manufacturing. As a Global Engineering Management she was responsible for research and development for Active ingredients and Formulation and process safety engineering. She led the development of computer models for physical property prediction, computer aided molecular design, process modelling and managing major partnerships between Syngenta and some of the world's top universities. Prof Cordiner chaired the 2021 report by the Royal Academy of Engineering for the Cabinet Office, working in collaboration with a select committee of the House of Lords on Improvements in the Processes for the National Security Risk Register. Joan's groups concentrate on modelling (mechanistic and data driven) of complex processes integrating process safety, maintenance and optimisation across a wide variety of processes from mRNA vaccines, pharm and chemical processes and fusion energy.

Digital Future of Chemical Industry- Challenges and Opportunities

Manufacturing processes can now be instrumented to provide rich data sets. From initial development of new processes through to operation and maintenance at scale the opportunities provided by data are vast. However, we still can't measure everything we need. This is where models are still needed whether that be for reactions, separations, properties, transitions states, polymorphic transformation and the like. By exploiting the benefits of mechanistic models, prediction techniques and machines learning we can develop hybrid models that can speed up development, improve manufacturing optimisation and operation and provide soft sensors for the things we can't yet measure. This is all critical to QbD and to reduce the cost monetarily in sustainability and in safety. Examples of such models and approaches will be presented for the different lifecycles stages of processes.

Nessa Carson

LinkedIn

Nessa completed her education at Oxford University and then the University of Illinois at Urbana-Champaign. She started off as a synthesis chemist in drug discovery for AMRI at Eli Lilly in Windlesham, then moved within the company to run the high-throughput automation facility, working across discovery and process chemistry. She then worked in high-throughput chemistry in process development at Pfizer in Sandwich, where she learned Python to optimize her team's workflows, before moving to Syngenta, to work with automation, data management, and workflow optimization. Nessa now works at AstraZeneca in Macclesfield UK, with the cool title of Associate Principal Scientist "Digital Champion". Nessa maintains a website of useful chemistry resources, https://supersciencegrl.co.uk.

Automate Your Own HTE Workflow

Attendees

In Person

Dr	Robin	Attrill	Consultant
Mr	James	Barber	AstraZeneca
Mr	Henry	Barrington	University of Strathclyde
Dr	Nathan	Barrow	Johnson Matthey
Miss	Molly	Bartlett	Imperial College
Dr	Andrew	Bird	Scale-up Systems Ltd
Mr	Will	Bowers	Dotmatics
Mr	Massimo	Bresciani	CMAC, University of Strathclyde
Mx	Nessa	Carson	AstraZeneca
Professor Dr	Mukund	Chorghade	THINQ
Professor	Joan	Cordiner	The university of Sheffield
Mr	Jeremiah	Corrigan	CPI
Dr	Bethan	Coulson	Johnson Matthey
Miss	Suzanne	Davies	GSK
Dr	Joe	Forth	University College London
Dr	Eugenie	Fournier	Euroapi
Mr	Robert	Gallen	Johnson Matthey
Ms	Julia	Gasol Cardona	CCDC
Mr	John	Gatenby	Dotmatics
Prof	Mike	George	University of Nottingham
Dr	Markus	Gershater	Synthace
Dr	Charles	Gordon	Scale-up Systems/Mettler Toledo Autochem
Dr	Alissa	Götzinger	DSM Nutritional Products AG
Dr	Thorsten	Gressling	Bayer AG
Professor	Mimi	Hii	Imperial College London
Dr	Mark	Hughes	Retired
Mrs	Rachel	Illsley	Mondelez International
Mr	Benjamin	Ingham	University of Manchester
Ms	Giada	Innocenti	hte GmbH
Dr	Alaa	Kadhim	Sphere Fludics
Dr	Phil	Kay	JMP Statistical Discovery
Ms	Amber	Keegan	University of Sheffield
Miss	Niki	Kotecha	Imperial College London
Dr	Stuart	Little	JMP
Miss	Erin	Maciejewski	GSK
Mr	Andrew	Maloney	CCDC
Mr	Edvin	Mamo	University College Dublin
Dr	Jade	Markham	Solvay
Mrs	Nicole	Mastrell	JMP Statistical Discovery
Dr	Timothy	McCabe	University of Strathclyde
Mr	Alexandru	Moldovan	Cambridge Crystallographic Data Centre
Dr	Oliver	Newton	GSK
Miss	Melanie	Nutter	Imperial College
Mr	Jerry	O'Reilly	Allied Bakeries part of Associated British Foods
Professor	Siddharth	Patwardhan	University of Sheffield

Mr	Peter	Rhodes	Dotmatics Ltd
Dr	Darren	Rhodes	Fine Organics Ltd
Dr	Lisa	Richards	Deepmatter Ltd.
Mr	Alexander	Rogers	The University of Manchester
Mr	Pietro	Sacchi	CCDC
Mr	Lluis	Sastre	Farmhispania, S.A.
Mr	Shainthavaan	Sathiyalingam	Imperial College London
Dr	Andrea	Sauerwein	Johnson Matthey
Mr	Linden	Schrecker	Imperial College London
Professor	Jon-Paul	Sherlock	AstraZeneca
Dr	Richard	Smith	2M Holdings Ltd
Dr	René	Stemmler	DSM Nutritional Products AG
Dr	Alan	Steven	CatSci
Mr	Fernando	Vega-Ramon	The University of Manchester
Miss	Haiting	Wang	Imperial College London
Dr	Sam	Whitmarsh	CatSci
Mr	Rob	Willacy	GlaxoSmithKline
Dr	Jason	Williams	Research Center Pharmaceutical Engineering GmbH
Ms	Luxi	Yu	Imperial College London
Ms	Ramona	Zaharia	Employee
Dr	Jiyizhe	Zhang	University of Cambridge

Online

Dr	Edith	Ciobanu	Syngenta
Dr	Stacy	Clark	GlaxoSmithKline
Dr	Liam	Donnelly	Strathclyde University
Mr	Zachary	Douglas	University of Nottingham
Mr	Calum	Fyfe	University of Strathcylde
Dr	Cristina	Garcia Morales	AstraZeneca UK
Mr	Richard	Hart	AstraZeneca
Dr	Hannah	Hayes	AstraZeneca
Dr	Nicholas	Jose	University of Cambridge
Dr	George	Karageorgis	AstraZeneca
Dr	Andrew	Mackey	Mondelez International
Dr	Kevin	Murphy	Astrazeneca
Dr	Patrick	O'Sullivan	Thermo Fisher Scientific
Mr	Enrico	Sangoi	University College London
Mr	Ralph	Sauer	The Sauer Consultancy Ltd
Dr	Carl	Steele	Atkins Limited / PCTG Honorary Chair
Miss	Emma	Thorpe	ALS Environmental
Dr	Simone	Tomasi	AstraZeneca
Dr	Ivalina	Tuxworth	Johnson Matthey
Dr	Toby	Waldron Clarke	AstraZeneca
Dr	Dongda	Zhang	University of Manchester

Posters

A case study on the application of design of experiments (DoE) and regression modelling to improve the productivity of sophorolipid biosurfactants.	Benjamin Ingham	University of Manchester
A Gaussian process-based hybrid modelling strategy for bioprocess kinetics simulation and uncertainty estimation	Fernando Vega-Ramon	The University of Manchester
A Hybrid Modelling Framework for Dynamic Modelling of Bioprocess	Haiting Wang	Imperial College London
A transfer learning approach for predictive modelling of bioprocesses using small data	Alexander Rogers	The University of Manchester
Applications of Computer Vision in Chemistry	Henry Barrington	University of Strathclyde
Chemical Process Automation Development	Edvin Mamo	University College Dublin
Combining Digitalisation with In-Situ Characterisation to Enable Improved Nanomaterial Synthesis: a Case Study on Silica	Amber Keegan	The University of Sheffield
Designing bioinspired green nanosilicas using statistical and machine learning approaches	Siddharth Patwardhan	University of Sheffield
Discovery of unexpectedly complex kinetic pathways for the Knorr pyrazole synthesis via transient flow	Linden Schrecker	Imperial College London
Ensemble Kalman Filter for estimation of intracellular nucleotide sugars from extracellular metabolites in monoclonal antibodies	Luxi Yu	Imperial College London
From simple formulations to real-world products: machine learning-based soft-sensor models to predict real-time viscosity	Jeremiah Corrigan	CPI
Innovation Centre in Digital Molecular Technologies	Jiyizhe Zhang	University of Cambridge
Probabilistic Machine Learning-based Soft Sensors for Product Quality Estimation in Batch Process Systems	Max Mowbray	The University of Manchester
Soft-Sensor design for monitoring and prediction of batch reactor operation and formulated product viscosity	Alexander Rogers	The University of Manchester
Using NLP on historical ELNs to determine reaction success or failure	Lisa Richards	Deepmatter

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- How to build better, cheaper solutions – by exploiting the deeper knowledge gained you can determine how to achieve optimum performance, consistently and at a lower cost
- How to reduce total experimental effort by 50% (often more) – by determining the best and minimal set of experimental combinations needed to address your questions upfront

Tip: Get even more out of this webinar

For a hands-on learning experience, download a free trial of JMP to follow along with the presenter.

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