Speakers: Dr Katharina Roettger, CPI & Rhys Kelly, M&I Materials

Title: *'Journey towards digital transformation: Leveraging historic data to optimise varistor manufacturing'*

Synopsis:

Existing manufacturing data often has untapped potential to solve long-standing production challenges and address inefficiencies. However, unlocking its value is often hindered by the fragmented formats, e.g. spreadsheets, handwritten notes, and legacy system logs. We will introduce CPI's COMPASS process to systematically map historic data to the manufacturing process. We will demonstrate its application to M&I's varistor production to highlight how targeted data exploration and planning can drive meaningful improvements and support digital transformation.

Biographies:

Dr Katharina Roettger is a Principal Scientist for Digital Technologies and Data Science at the Centre for Process Innovation (CPI). Katharina has over 10 years of experience working with industrial and academic partners in the manufacturing sector. Her focus is on using existing site and process data for more efficient material development as well as product and process optimisation to make the UK manufacturing sector more competitive and sustainable.

Rhys Kelly is a Process Development Technologist working at M&I materials, a specialist materials manufacturer in Trafford Park, Manchester. Having worked at M&I for almost 3 years, transitioning from a laboratory technician to the role he sits in now; Rhys creates and runs projects which focus on improving quality and throughput and reducing waste, utilising a methodical and wholeheartedly collaborative approach to ensure immediate and sustainable success within the business.

Speaker: Dr Carl Tipton, Johnson Matthey

Title: *'Industrial IOT in the Process Sector: a Case Study'*

Synopsis:

In this talk we discuss the process of converting a laboratory scale measurement technique into an industrial grade instrument for use in a manufacturing environment. The novel instrument uses acoustic emission to detect air entrained in Johnson Matthey Products. The low-cost sensor discussed generates information rich time series data. The development challenge initially centres on the creation of a robust novel algorithm using the Hilbert Transform, a Savitsky-Golay filter, and peak detection. The results of an onsite trial of the prototype solution is then presented. In the second half of the talk the design process of creating a robust piece of equipment for use in a manufacturing site will be discussed alongside the further refinements of the algorithm required. Considerations such as ergonomics, data connectivity, data formats and data safety will be presented.

Biography:

Carl studied Physics with Theoretical Physics at the University of Manchester in the late 90s. He then continued his studies in Manchester and completed a PhD in Nonlinear Physics with Prof Tom Mullin. He then did a one year Post-Doc in Eindhoven with Prof. Willem van de Water. These were very all experimental projects, and they revealed that he was probably more interested in how to measure things than what he was actually measuring. A 5 year stint in transport planning consultancy followed, where he built up skills in database design and software development and notably developed strategic passenger modelling software for the US Federal Aviation Administration. (Transport planners were doing big data analysis before it was a buzz word). In 2010 Carl returned to academia in Manchester before joining the Johnson Matthey Business, Tracerco, in 2013. Here he developed industrial instrumentation and started to bring together the measurement and database skills together, whilst learning about the importance of industrial standards. He moved to Johnson Matthey Technology Centre in 2019 has been bringing all these skills together to deliver novel Industrial IOT solutions to the Johnson Matthey production plants. He has 10 granted patents in this space.

Speakers: Dr Meera Shah, Mitsubishi Chemical UK and Adam Wilson, KEIT.

Title: *'Application of online process analytics to the Alpha MMA process'*

Synopsis:

Successful implementation of the Keit IRmadillo analyser technology to MCUK's Alpha MMA production process. The talk highlights how real-time compositional analysis using advanced IR technology enables rapid, accurate monitoring of complex chemical streams, overcoming the limitations of traditional offline methods.

Biography:

Meera Shah: I am a Senior Research Scientist at Mitsubishi Chemical UK. My career has developed through a blend of academic and industrial research, beginning with an MSci in Natural Sciences and a PhD in Chemistry from Durham University, where I explored methane activation using zinc-modified zeolites. I completed a postdoc at KU Leuven, working on CO_2 valorisation and advanced material characterisation. In industry, I started as a research scientist in the polymer team where I led R&D projects in polymer development, including medical-grade PMMA. My research is now focused on MMA catalyst development and recycling.

Adam Wilson: After obtaining my PhD in supramolecular chemistry from the University of Edinburgh, I worked on various academic projects researching oligonucleotide synthesis and exotic intermolecular forces. Since then I have moved into industry, where I have transitioned away from the lab and into statistical and data science roles. I have worked in the synthesis of chromatography gels; in medical microfluidics devices; and in bioinformatics. I now work at Keit Industrial Analytics, where I am exploring the use of real-time mid-infrared spectroscopy and chemometrics to optimise factory operations across the chemical and bioethanol industries.

Speaker: Dr Sourav Chatterjee, The University of Bath

Title: *'From Bench to Algorithm: Teaching Digital Chemistry to the Next Generation of Chemists'*

Synopsis:

As chemistry undergoes a digital transformation, the demand for chemists fluent in data science, machine learning, and automation is rapidly growing. In this talk, I will reflect on my experience designing and delivering digital chemistry training through academic courses and industry-facing workshops, including the widely attended "Empowering Chemists with AI and ML: Transformative Tools and Techniques" course delivered with Scientific Update. I will explore the challenges of introducing data-centric thinking to experimental scientists, highlight common misconceptions, and share insights into what pedagogical strategies have worked, and what haven't. Key focus areas will include identifying core competencies in digital chemistry, structuring accessible training for beginners, integrating case studies to bridge theory and application, and developing metrics to evaluate learning outcomes. The goal is to provide a practical perspective for educators, industrial leaders, and policymakers seeking to build effective digital chemistry training programs that prepare chemists for the demands of tomorrow's labs.

Biography:

Sourav's research interest lies in the design and application of Automation, flow chemical systems and Machine Learning to understand and study complex chemical problems. He obtained his MSc (with distinction) and PhD from Queen`s University of Belfast, UK for the design of radiofrequency heated microreactor for fine chemical synthesis. His research was highlighted in the cover of Chemical Engineering Journal. He subsequently received postdoctoral research fellowship from Max Planck Society in Germany and continued his research in Max Planck institute of Colloids and Interfaces in Potsdam. There he developed automated flow chemical platforms for controlling chemical glycosylation and multistep organic synthesis. He applied machine learning algorithms combined with computational chemistry and automated platform to predict stereoselective outcome of chemical glycosylation. Finishing his postdoctoral research, he moved to ETH Zurich as a Team Leader of Automation and AI in chemistry and catalysis. He helped developed machine learning workflows for Swiss Catalysis Hub East at ETH Zurich and obtained research grant at ETH Zurich from NCCR Catalysis. From February 2023, Sourav began his independent academic career as a Lecturer (Assistant Professor) in the Department of Chemical Engineering at University of Bath and currently is the principal investigator of AI/ML guided automated flow synthesis laboratory at Bath. He has won the Best Oral Presentation award at the ChemEngDay UK 2023 conference and has worked on research projects funded by ERC and DARPA. He has published his research in several prestigious scientific journals like JACS, Chemical Engineering Journal, Chemical Science and Nature.

Speaker: Dr Dongda Zhang, The University of Manchester

Title: *'AI Lessons from Discovery Models to Molecule Generation: Scaling Intelligence Across Process Chemistry'*

Synopsis:

In this talk, I will share insights from my Royal Academy of Engineering Industrial Fellowship with Unilever, focusing on how predictive and generative AI can scale intelligence across process chemistry. The presentation will cover interpretable AI and augmented intelligence for knowledge discovery, digital twin construction, and process optimisation, alongside statistical and probabilistic machine learning methods for pattern recognition and product quality monitoring. Advances in AI foundation models for inverse molecule design and property prediction will also be highlighted. Applications spanning plant-scale operations to molecule-level design will illustrate both the challenges and the opportunities of digital innovation across small- and large-data scenarios.

Biography:

Dr. Dongda Zhang is a Lecturer in Process Systems Engineering and Machine Learning at the University of Manchester, and a Royal Academy of Engineering Industrial Fellow with Unilever. His research integrates chemical engineering, artificial intelligence, and digital manufacturing, with a focus on interpretable machine learning, hybrid modelling, and data-driven optimisation. Through his industrial fellowship, which supports Unilever's digital expansion and cultural transformation, Dr Zhang has developed advanced AI solutions for process flow diagram optimisation and scale-up, knowledge discovery, factory-level product quality monitoring, molecular property prediction, and inverse material design. At this meeting, he will share lessons learned from deploying diverse data intelligence tools and discovery models across process chemistry workflows – from plant-scale implementation to molecule-level design – highlighting practical challenges and scalable opportunities in digital innovation.

Speaker: Dr Adam Clayton, The University of Leeds

Title: *'The Chemist of the Future'*

Synopsis:

As digital and automated technologies transform the landscape of chemical research, we face a critical question: do we have the right people with the right skills to drive this change? In this talk, I'll explore the training pipeline for the next generation of digital chemists, including where the key skill gaps lie, and how we can design programmes that prepare students for this rapidly evolving field. Drawing on my experience developing the MSc in Digital and Automated Chemistry at the University of Leeds, I'll share what we've learned about building interdisciplinary expertise that blends chemistry, data science, and automation. I'll also draw on examples from my own research in digital chemistry to illustrate how these technologies are reshaping both the way we do chemistry and the kinds of skills our students need to thrive.

Biography:

Dr Adam Clayton comes from Huddersfield, in Yorkshire, and completed an MChem in Chemistry at the University of Huddersfield in 2016. He was then awarded an AstraZeneca CASE studentship to study a PhD with Professor Richard Bourne at the University of Leeds, working on the development of multi-objective self-optimising continuous flow reactors. He received his PhD in 2020 and then joined the Institute of Process Research and Development as a postdoctoral researcher to continue developing autonomous workflows for process optimisation. During this position he established new digital approaches to accelerate pharmaceutical process development and integrated these technologies within the labs of multiple industrial collaborators.

Dr Clayton was awarded a Royal Academy of Engineering Research Fellowship in 2022 to investigate the 'Autonomous Development of Telescoped Catalytic Reactions' at the University of Leeds, where he has been an Associate Professor of Digital Chemistry since 2024. His research interests are focused on developing efficient and more sustainable multistep processes in continuous flow, principally for small molecule synthesis. To achieve this he designs and utilises machine learning algorithms to guide experimental campaigns performed on autonomous reactor platforms. Dr Clayton is also the Programme Manager for the MSc in Digital and Automated Chemistry course at the University of Leeds.