

Tuesday 16th January 2024 **Sustainability** Agenda

	DETAILS
09:30	Arrival and registration with refreshments.
10:00	Opening remarks: Introduction and outline of the day from John Arthur, Centre. Foreword from Laura Kelly (PwC).
10:30	Session 1 begins: <b>Chemistry</b>
	<ul> <li>Graeme Barker (HW) - Flow Chemistry</li> <li>Cameron Webster (Pluto Mills LTD) - Mechanochemistry</li> <li>David Nelson (CataNiTek) - Nickel catalysts</li> </ul>
11:30	Break and opportunity to meet Session 1 innovators
12:00	Session 2 begins: <b>Processes</b>
	<ul> <li>Marc Reid (UoS) – Reaction monitoring</li> <li>TBC</li> </ul>
	Patryk Kujawa (CPI) - Sustainability programmes at CPI
13:00	Lunch and opportunity to meet Session 2 innovators
14:00	Session 3 begins: <b>Technology</b>
	<ul><li>Ben Pellegrini (Intellegens)</li><li>Jamie Young (EECO2)</li><li>Iain Crosley (XpertRule)</li></ul>
15:00	Break and opportunity to meet Session 3 innovators
15:30	Review of the day with concluding thoughts from John Arthur, CPI
16:00	Networking session
16:30	Event close



Director of CPI's Medicines Manufacturing Innovation



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## Graeme Barker, Heriot-Watt University Tales from the Continuum Flow Lab

The Continuum Flow Lab is a recently established facility based at Heriot-Watt University dedicated to continuous flow reaction monitoring. Continuous flow chemistry is well-established as offering significant advantages in terms of energy efficiency and process safety, as well as offering more precise control of reaction timings and temperatures than traditional batch synthesis and inherently easier scalability. The Continuum Flow Lab offers a wide suite of continuous flow synthetic capabilities married to cutting-edge reaction monitoring instrumentation and a broad spectrum of academic expertise (see below). We aim to offer access to external industrial and academic users who wish to engage with flow chemistry but currently lack the resources to do so independently, are already active in flow chemistry and wish to explore advanced reaction monitoring techniques or require additional expertise or staff experience to fully exploit this rapidly emerging field.

To showcase the capabilities of Continuum, several case studies of recently published academic research carried out in the facility will be presented, including continuous flow C-H functionalisations of common pharmaceutical moieties, in-line benchtop NMR for optimisation of additive manufacturing, 3D printing of photocatalytically active reactors, and the first example of continuous at-line purifications using normal phase chromatography.

Contact: Facility Inbox: continuum@hw.ac. Dr Graeme Barker (synthesis in flow, continuous purifications): graeme.barker@hw.ac.uk Find out more

#### David Nelson and Elliot Johnson Humphrey, CataNiTek Novel Nickel Catalysts for Fine Chemicals Synthesis with Lower Environmental Impact

Precious metal catalysts are ubiquitous in pharmaceutical manufacture for their stability, predictable behaviour, and wide scope. A very large number of drugs are manufactured using a palladium catalyst for at least one synthetic step. However, palladium is found in areas that often have significant geopolitical risk, with ca. 80% of production coming from Russia and South Africa. Palladium is expensive and, as a result of its low natural abundance, its production and refinement is highly polluting; approximately 7 to 20 kg of CO2 equivalents are produced per gram of palladium.

Nickel offers an attractive alternative: it is much more abundant, is found in multiple countries on each continent, is considerably less expensive, and is much less polluting. The production of a gram of nickel generates fewer than ten grams of CO2 equivalents. Nickel can replace palladium in many reactions, and can perform a range of chemical reactions for which palladium is not competent.

The uptake of nickel catalysis in industry is limited by the lack of robust, well-defined, and commercially available nickel catalysts. CataNiTek, a forthcoming spin out from the University of Strathclyde, has developed a series of patent-protected complexes that have considerable potential as catalysts for chemical manufacture. These can be prepared with a wide variety of structures, and so can be tuned for specific applications. They initiate rapidly and irreversibly under reaction conditions, and our initial benchmarking has shown them to be up to twice as effective as alternative nickel catalyst systems.

Find out more





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# Cameron Webster, Pluto Mills LTD Mechanochemistry and Planetary Ball Mills

A brief introduction to Mechanochemistry while highlighting the multiple green credentials. A walkthrough of planetary ball mills and the current offer from Pluto Mills LTD while outlining the opportunity of mechanochemistry for sustainability and business.

Find out more

# Marc Reid, The University of Strathclyde Kineticolor: Non-contact Reaction Monitoring with Computer Vision

Chemistry research is dominated by colour changes, both subtle and stark. At the same time, few reaction monitoring tools can be used on both small and large scales. With cameras and computer vision, the hardware and software needed for more time-, cost-, and safety-effective monitoring of high-value chemical processes can be realised. In this seminar, the reaction monitoring video analysis platform Kineticolor will be introduced. The technology is part of a prospective spinout from the University of Strathclyde. Kineticolor provides a rare and chemistry-agnostic example of a non-contact analytical tool that can provide quantifiable insights on reaction bulk. It complements the large suite of more specific analytical tools (mainly in situ probes) used to analyse small and intermediate-scale reaction systems. Applications include catalyst activation, deactivation, material photodegradation, forensic spot testing, amidation, and process-scale mixing analysis.1-4 In discussion, we invite collaborations with end users whose research would benefit from reaction monitoring by a means that requires no intervention to how their processes are currently set up.

Find out more





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### Patryk Kujawa

#### **Sustainability at The Medicines Manufacturing Innovation Centre**

CPI is committed to sustainability in all its activities, and this session will show you how we are implementing this commitment in our Medicines Manufacturing Innovation Centre. Our senior management has set a clear direction and vision for us to become carbon-neutral by 2030, and we are working hard to achieve this ambitious goal. You will learn how our facility design incorporates sustainability principles, such as energy efficiency or renewable sources. You will also see how our Grand Challenges align with sustainability objectives, such as using less solvents, reducing waste and improving process efficiency. We hope this session will inspire you to join us in our journey towards a greener future.

### Iain Crosley, XpertRule Sustainability a challenge or an opportunity

With the pharmaceutical sector accountable for an estimated 4.4% of worldwide emissions, pharma manufacturers are struggling to meet Net Zero and sustainability targets while maintaining their competitive edge.

Our integrated, intuitive manufacturing platform enables process engineers to raise quality, optimise operational efficiency and increase uptime - all while complying with increasingly stringent regulations.

By better optimising production patterns with real-time condition monitoring, process modelling and anomaly detection, pharma manufacturers can increase uptime by 15%, reduce energy usage, and emissions and make huge steps towards Net Zero. All while improving machine visibility and audibility to not only comply with but go above and beyond regulatory obligations.

As a customizable AI product, use cases for XpertFactory in the pharmaceutical sector cover all areas, from R&D, to formulation, production, packaging and even looking to designer medicines in the future. As the industry heads toward continuous manufacturing, companies will need more data, better machine visibility, data-driven rules and process insights to allow quality by design (QBD) and process analytical techniques (PAT) to be applied.

All in an auditable and highly visible format and not a "black box".

Find out more





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## Ben Pellegrini, Intellegens Separating ML hype from reality: Addressing the Sustainability Challenge

This talk focuses on the use of machine learning (ML) for data analysis and optimising experiments, products, and processes in research-intensive and manufacturing industries. We will introduce Intellegens, the sustainability challenge and how we think about machine learning, followed by a focus on practical applications proven through real case studies.

Delivering cost and performant solutions is already a complex, multi-parameter optimisation problem. The increasing need to meet sustainability and net zero targets makes this task yet more challenging. Machine learning (ML) can help extract added value from all available data to propose new designs and processing options and to guide experimental programs. We will discuss the use of ML for a range of sustainable material, chemical and formulation design and development challenges with real-world, proven case studies.

#### **Find out more**

### Nick Bancroft, EECO2

**Smart Cleanrooms: Utilising Demand-Based Control for Sustainable Facilities** 

For decades, the approach to cleanroom air changes has remained the same. Airflow provided to the space remains at a static level, with no regard for the amount of activity in the space or the contamination challenge at any given point â€" missing a significant opportunity for air change rate reduction.

Utilising a dynamic approach (named ICCS) that embraces modern particle counter technology, dynamic cleanroom control now allows a facility to react to the particle generation rates within a cleanroom space and only provide the required airflow depending on this demand.

Our presentation will use real-life data from the first commercial implementation of this concept to demonstrate how this technology performs from a quality and compliance standpoint, as well as the associated energy reduction and sustainability benefit.

#### **Find out more**



