UNIVERSITY OF SURREY

DIGITALLY ENABLED CIRCULAR ECONOMY

WORKSHOP PROGRAMME

2 May 2024

OUR SPONSORS

Institute of Advanced Studies

The Institute of Advanced Studies (IAS) at the University of Surrey sponsors workshops and Fellowships at the 'cutting edge' of science, engineering, social science and the humanities. Through this scheme the Institute fosters interdisciplinary collaborations and encourages a flow of international scholars to visit, enjoy their stay at Surrey and leave behind excellent ideas and innovations.

ias.surrey.ac.uk

UKRI Interdisciplinary Centre for Circular Chemical Economy

The National Interdisciplinary Centre for the Circular Chemical Economy (CircularChem) brings together stakeholders from academia, industry, government, NGOs and general public to transform the UK's chemical industry into a fossil-independent, climate-positive and environmentally-friendly circular economy. As part of a £30 million strategic government investment it will play a key role in helping the UK to reduce waste and the environmental impacts of production and consumption and creating opportunities for new UK industries.

circular-chemical.org

OXCCU

OXCCU is a spinout company from University of Oxford based on more than 10 years research in the Inorganic Chemistry Laboratory, focusing on the catalytic technology to convert CO2 and hydrogen into aviation fuel and chemicals to achieve circular economy. Our 1-step CO2 catalytic hydrogenation to sustainable aviation fuel is the world leading technology economically enabling CO2 to be feedstock for net zero world. So far, OXCCU has raised more than 20 million pounds, including investments from IP group, Clean Energy Venture, United Airline, ENI, Saudi Aramco, Trafigura and so on.

oxccu.com

INTRODUCTION

University of Surrey, in collaboration with the Alan Turing Institute, CircularChem, and OXCCU, is hosting an interdisciplinary workshop focused on implementing digital technologies, such as digital twins (DT), to enhance the circular economy within UK industries. This workshop aims to promote sustainable growth in the UK's manufacturing sectors, with the overarching goal of achieving Net Zero emissions. By transitioning from linear production to a circular economy model, digitalisation serves as a key facilitator in this shift. The workshop will provide a platform for experts from diverse fields, including engineering, data science, business, and social sciences, to share innovative ideas, best practices, and explore potential collaborations, thereby driving forward knowledge exchange in digitally enabled circular economy initiatives.

Workshop Chairs:
Dr Lei Xing and Dr Regina Frei (University of Surrey)

Organising committee:
Professor David Wagg (University of Sheffield) and Dr Tiancun Xiao (OXCCU, University of Oxford)

Administrative support:
Louise Jones (Institute of Advanced Studies) and Zhilin Yang (University of Surrey)

PROGRAMME

THURSDAY 2 MAY
Treetops, Wates House

(BST)	
09.00 – 09.30	Registration
09.30 – 09.45	Welcome and Introduction Lei Xing, Regina Frei, David Wagg and Tiancun Xiao
	Session 1: Lei Xing (Chair)
09.45 – 10.15	The Philosophical Foundations of Digital Twins Professor David Wagg (Alan Turing Institute)
10.15 – 10.45	Role of Digital Tools in Sustainability Assessment of Early-Stage Chemical and Fuel Technologies Professor Benoit Chachuat (Imperial College London)
10.45 – 11.15	Digital R&D, Digital Engineering, and Digital Operations for Circular Economy Dr S. Phil Han (Siemens)
11.15 – 11.45	Accelerating Transition Towards a Circular Chemical Economy: A Systems Perspective Professor Bing Xu (Heriot-Watt University)
11.45 – 12.00	Break & Photographs
12.00 – 12.45	Panel Discussion Professor Jin Xuan, Professor David Wagg, Professor Nik Watson, Professor Eileen Yu, Professor Bing Xu, Dr S. Phil Han, Robert Purchase, Fajli Bib
12.45 – 14.00	Lunch and Poster Presentations
	Session 2: Regina Frei (Chair)
14.00 – 14.30	Enhancing Agri-Food Transparent Sustainability (EATS) Professor Nik Watson (University of Leeds)
14.30 – 15.00	Digitalisation: A Path to Resource Efficiency Professor John Ahmet Erkoyncu (Cranfield University)
15.00 – 15.30	Using Simulation to Evaluate Circular Supply Chains of Small Medical Devices Professor Antouela Tako (Nottingham Trent University)
15.30 – 16.00	Stabilising Systems for Sustainability Equilibrium through Industrial Autonomy Robert Purchase (Yokogawa)
16.00 – 16.30	Break
	Session 3: Ideation workshop (5 groups) **Co-chairs: Lei Xing, Regina Frei, Xiaoxue Shen, Oliver Fisher and Miao Guo**
16.30 – 17.30	How does digital technology interact with the circular economy to foster mutual development? Topic 1: How digital twin technology can be leveraged to optimise circular economy processes and promote circular economy business? Topic 2: How circular economy approaches can be applied on digital technologies to maintain their sustainable development? Topic 3: How IoT infrastructure and cyber security would be applied to support the digitally enabled circular economy?
17.30 – 18.30	Networking Reception
19:00 – 21.00	Dinner

ABSTRACTS AND PARTICIPANTS

Professor David Wagg

David's research interests are focused on improving the performance of engineering systems. For a significant number of applications, including wind power, land transport, aerospace and large civil infrastructure, dynamic effects can dominate the operational performance regime. His current research activities are focused on developing techniques for the design, implementation and interoperation of digital twins for engineering applications. Quantifying uncertainties within a dynamic digital twin context is a major topic of interest. Uncertainty (and trust) relates to the overall objective of validating the outputs of a digital twin. Other topics of interest include modelling emergent behaviours, developing software & hardware platforms for digital twinning, and using ontological knowledge models for interoperation between digital twins.

The Philosophical Foundation of Digital Twins

Professor David Wagg (Alan Turing Institute)

Digital twins offer the possibility of interconnected virtual representations of the world around us. The digital twin concept has been adopted widely by multiple communities of practitioners, researchers and innovators. In particular policymakers and governmental agencies have identified digital twins as having many potential applications offering a wide range of societal benefits. Part of the digital twin paradigm is about interconnecting and integrating digital objects, many of which have previously not been combined, often to address socio-technical applications. The different starting points, assumptions, cultural practices, biases and motivations of those involved, means that discussions across the socio-technical sphere are often at cross-purposes and without a common philosophical world-view. Therefore, the philosophical context which underpins the concept of digital twins is an important area to make clear. This leads to a set of philosophical principles for digital twins, which are intended to help facilitate their further development. We argue that the philosophy of digital twins is fundamentally holistic (e.g. anti-reductionist). Furthermore, digital twins are reconstructivist, meaning they are designed to reconstruct (some or all of) the behaviour of a physical twin by assembling a series of ``components'', such as models, agents and data sets. Importantly, these digital twin components have the potential to capture emergent behaviours when they are dynamically assembled. Understanding the philosophical principles allows key questions to be investigated.

Continued ▶

Professor Benoit Chachuat

Benoit Chachuat is a Professor of Process Systems Engineering at Imperial College London and Director of Research at the Sargent Centre for Process Systems Engineering. His primary research focus is on the development of new methods and tools for modelling and optimization of complex process systems. Current application areas in his research group include sustainable chemical and low-carbon fuel production, and quality-by-design in pharmaceutical manufacturing. He is leading the theme on 'Process integration and whole systems optimization' of the UKRI Interdisciplinary Centre for Circular Chemical Economy.

Role of Digital Tools in Sustainability Assessment of Early-Stage Chemical and Fuel Technologies

Professor Benoit Chachuat (Imperial College London)

The ability to assess the economic and environmental performance of early-stage technologies at production scale is critical for sustainable future process development. This presentation starts by reviewing the benefits of combining detailed digital simulation tools with available costing and environmental impact databases to support such early-stage technology assessment. A comparison of alternative pathways to ethylene production at various technology readiness levels and from various carbon feedstocks and energy sources is used as an illustrative case study. The need for further methodology and software development is then discussed, including automating the workflows for flowsheet construction and energy integration; conducting systematic uncertainty quantification and sensitivity analyses for guiding further experimental efforts; and challenges arising from assessing the economic and environmental impact of novel catalysts and sorbents.

Dr Sang Phil Han

Sang Phil Han is the head of Competence Centre Process Modelling, Siemens Process Automation Software. Prior to this role, he was the head of BU E&C, Siemens PSE, President of PSE Korea, PSE APAC, Project/team leader of LG Chem R&D. He got his BS, MS and PhD degree in Chemical Engineering from KAIST. His areas of expertise and experience are Advanced Process Modeling (APM) based on multi-scale and multi-physics hybrid simulation technology, especially via coupling of gPROMS® and CFD, and physics-based models and data-driven models, APM based experiment design, processing unit design, plant process design, and operational excellence solutions for process industries.

Digital R&D, Digital Engineering, and Digital Operations for Circular Economy

Dr Sang Phil Han (Siemens)

The multifaceted crisis caused by climate change has been calling for prompt and effective transition from the linear economy to the circular economy across all industries. A circular economy prioritizes developing and producing products that generate minimal waste during production and usage. It also aims to minimize the impact of the industrial actions on the environment by making the products return to the earth harmlessly or convert to reusable resources and products. Process industries are producing crucial products to keep and enhance the quality of life for all mankind but also are one of the major contributors to carbon emission. So, the transition of process industries to circular economy is very important but extremely challenging, and it requires the development, application, and adoption of new technologies, processes, and plants in the most effective and efficient way. Siemens Process Automation Software division is offering variety of digitalization solutions to combine the real and the digital worlds to help customers remain competitive, resilient, and sustainable throughout the whole product and process lifecycle under this highly dynamic and demanding circumstances all around the world. This presentation will focus on how 3 different digital twins – Process Digital Twin, Plant Digital Twin, and Automation Digital Twins - can be utilized, respectively and together, to maximize the effectiveness and efficiency in developing new products and processes from R&D, through engineering, to operations, and also to transform and optimize existing plants in operation. Several cases about design, engineering, and operation of key processing unit (e.g. reactor) and whole plants for chemicals, pharmaceuticals, hydrogen, polymers will be presented in the aspect of how data and models can be combined and utilized seamlessly to make innovation transform the process industries towards the green circular economy.

Continued ▶

Professor Bing Xu

Bing is a Professor of Finance, the Business & Finance Theme Lead at the Institute for Net Zero and Beyond (iNetZ+), Heriot-Watt University. She holds an MA (Hons) in Business Studies & Accounting and a PhD in Management, both from the University of Edinburgh. Her research focuses on leveraging social science innovations to tackle the challenges of achieving net zero, particularly in the areas of low carbon fuels, and circular economy. Currently Bing leads "Policy, Society and Finance" theme of work on several UKRI funded projects to address barriers around business and finance models, social dynamics, investment and policy decisions., PSE APAC,

Accelerating Transition Towards a Circular Chemical Economy: A Systems Perspective

Professor Bing Xu (Heriot-Watt University)

Despite widespread recognition of the circular economy (CE) concept, its implementation in the chemical manufacturing industry remains challenging. Our research focuses on the non-technological obstacles that impede the broader adoption of circular practices, aiming to catalyse the transition to a CE. Specifically, we aim to provide an in-depth understanding of how embracing circularity influences business models and analysing the motivating factors driving businesses and financiers to align their efforts with CE principles. Furthermore, we capture public knowledge, perception, attitudes, and willingness to pay towards sustainable products. Through scenario experimentation, we investigate the interconnections between key policy measures and behavioural factors. This helps us pinpoint turning points in the transition to circular economy. In addition, we propose novel network approaches to assess the circular economy performances.

Professor Nicholas Watson

Nik is a Professor of Artificial Intelligence in Food in the School of Food Science and Nutrition at the University of Leeds. His research is focused on developing digital technologies and solutions to address environmental sustainability, food safety and health challenges in food production systems. His particular expertise lies within combining low costs sensors (e.g. acoustic and optical) with machine learning models to monitor and optimise production processes and predict food properties. Nik is a Chartered Engineer with a MEng in Mechanical Engineering (University of Hull, 2006) and PhD in Chemical Engineering (University of Leeds, 2010). From 2010 - 2014 Nik worked as a Post-Doctoral Research Assistant in the Food Physics Lab at the University of Leeds and from 2014 - 2023 Nik was an Assistant/Associate Professor of Chemical Engineering at the University of Nottingham.

Enhancing Agri-Food Transparent Sustainability (EATS)

Professor Nicholas Watson (University of Leeds)

The UK has a legally binding target of 'net zero' greenhouse gas (GHG) emissions for 2050 (Scotland, 2045) and the Food and Drink sector has a vitally important role to play in helping to achieve this. This must be done while also improving nutrition, protection of ecosystems, reduced risks to soil, water and air quality. Delivery against these ambitious targets will require a range of measures to be adopted across the agri-food supply chain - not just primary producers but also processors, retailers and ultimately consumers. Over the last few decades rapid advances in processes to collect, monitor, disclose, and disseminate information (broadly classified under the concept of 'transparency') have contributed towards the development of entirely new modes of environmental monitoring and governance for supply chains.
Unfortunately, existing approaches often suffer from limitations in terms of collection and dissemination of data; over-simplification of supply chains; power dynamics influencing information inclusion/exclusion decisions; and potentially perverse outcomes regarding how the information is used, by whom and to what effect.
Given these issues, we need to consider how best to capture information about supply chains in order to document existing sustainability practices in sufficient detail; this is necessary to not only support monitoring and reporting needs of all stakeholders, but also to

Continued ▶

promote additional pro-environmental behaviours and even re-configuration of the supply chain. Our vision is built around an actionable information ecosystem whose purpose is to deliver transparent sustainability - realised via three pillars that we refer to as: SEE-SHARE-ACT. The first of these encompasses the role of sensors and carbon reporting tools in capturing data about agri-food processes (SEE); the second is a trusted digital platform able to manage sustainability data and report it across supply chain actors (SHARE); the third is the use of data-analytics and machine learning to support decision-making and action (ACT).

Professor John Erkoyuncu

John A. Erkoyuncu is Professor in Digital Engineering and Head of the Centre for Digital Engineering and Manufacturing at Cranfield University. His research interests include: digital twin, augmented reality, and digitalisation of through-life support. He has a track record in leading research worth over £8M through EPSRC (most recent – PI: EP/R013950/1, Co-I: EP/R032718/1), Innovate UK, and EU. He has published over 160 scientific papers. John is Co-Chair of the Through-life Engineering Services Council, Community Council Member of the Digital Twin Hub, Chartered Engineer with IET, Fellow of HEA, and Associate Fellow of CIRP. John is the Course Director for the MSc in Digital and Technology Solutions.

Digitalisation: A Path to Resource Efficiency

Professor John Erkoyuncu (Cranfield University)

This presentation is aimed at providing an overview of how digital technologies such as digital twins can lead to improved process efficiency and better use of resources. the talk will explore alternative uses of digital technologies, and provide examples on how resource efficiency can be improved. The talk will reflect on emerging research opportunities, and areas that could be beneficial for a resource efficient future.

Professor Antouela Takou

Antouela is Professor of Operations Research at Nottingham Business School, Nottingham Trent University. Her research focuses on alternative simulation approaches, facilitated simulation, systems thinking and behavioural operational research. Anotuela is an expert in developing approaches to support stakeholder engagement in model-based interventions, primarily in healthcare. She is co-founder of the PartiSim approach and a Co-Investigator on the EPSRC-funded project, Re-Med (Circular Economy of Small Medical Devices). She is Associate Editor of the Journal of the Operational Research Society, Journal of Simulation, Area Editor of Health Systems Journal and a member of the EPSRC Peer Review College.

Using Simulation to Evaluate Circular Supply Chains of Small Medical Devices in Healthcare

Professor Antouela Takou (Nottingham Trent University)

Simulation can play an important role in developing digitally enabled circular economy systems. This presentation provides an overview of the ongoing modelling work currently being undertaken as part of an EPSRC-funded project called ReMed (ciRcular Economy for small Medical Devices). Our models aim to evaluate the impact of introducing circularity in the supply chains of small medical devices (SMDs) by comparing different scenarios of a circular economy against a linear economy system. We use AnyLogic to build simulation models that represent the flow of SMDs through a network of supply chain members (manufacturers, distributors, NHS providers, and re-processors) and their interconnections. The implications of transitioning to a Circular Economy-based system are assessed through economic, operational and environmental performance indicators. For illustration purposes a model of an example small medical device, laparoscopic scissors, and the results of some preliminary what-if scenarios are presented.

Robert Purchase

Robert Purchase is a mechanical and marine engineer with over 25 years' experience in engineering service, sales. For the last 10 years he has worked in automation & instrumentation project delivery and business development. Now responsible for Strategy & Sustainability at a global Industrial Automation corporate he rationalises the systems convergence of technological strategy and sustainability in critical industry and infrastructure. He is a certified ISO9001, ISO45001 & ISO14001 auditor and ISO44001 and ISO50001 lead implementor.

Stabilising Systems for Sustainability Equilibrium through Industrial Autonomy

Robert Purchase (Yokogawa)

In 2017, Yokogawa set out its three sustainability goals. We would "Work to achieve net-zero emissions by 2040, ensure the well-being of all, and make a transition to a circular economy by 2050, making the world a better place for future generations." However, the associated challenges are so complex the need for an understanding individual component parts and the wider system is no longer a luxury, but a critical necessity. Beginning with the inception of Systems Engineering in 1947 and the first digital computer. From the Servomechanisms Lab at MIT where Jay Forrester began work on a machine that would come to be known as Whirlwind, to the use of artificial Intelligence embedded industrial edge computing available today, I propose that in order to stabilise the volatility of global market forces and voracious energy consumption we must transform our linear materials model to a circular one. To tackle the process and scientific challenges required to realise this and unlock the knowledge currently bound by archaic, repetitive manual tasks, we must leverage Industrial Autonomy.

POSTER PRESENTATIONS

Electrochemical CO_2 Reduction to Chemicals: Challenges to Industrial-Scale Implementation
Bhavin Siritanaratkul (University of Liverpool)

Powered by renewable electricity, electrochemical CO_2 reduction is a promising pathway to convert CO_2 into valuable fuels and chemicals, thus creating a circular flow of carbon feedstocks. Here, we highlight barriers to implementing industrial-scale CO_2 reduction, including catalyst and cell stability, voltage losses, impurities in real-world feed CO_2, and downstream separation requirements.

Creating Net Zero Circular Economy via Waste to Energy and Resource Transformation
Hui Luo (University of Surrey)

In the transition towards Net-Zero, there is significant interest in phasing out fossil fuels as both the energy source and precursor for petrochemicals. Biomass is recognised as an ideal CO_2 neutral, abundant and renewable resource substitute to fossil fuels. The rich proton content in most biomass derived materials endows it to be an effective hydrogen carrier. The inherent chemical structure allows them to be easily catalysed to produce valuable commodity chemicals that can be used in applications such as biodegradable polymers and pharmaceuticals. Although historically biomass has been regarded as waste stream, recent years have seen increasing attentions in valorising it into useful products.

Looking beyond, beside utilising biomass, an even higher urgency lies in recycling the accumulating plastic waste into useful products. Mechanochemistry has emerged as a safe, efficient and green technique. Using just mechanical energy, this process can cleave chemical bonds and depolymerise long-chain molecules such as cellulose and plastics, revealing huge potential in industrial applications. By transforming a liquid process into a solid-state reaction, this technique can also significantly reduce solvent consumption. Therefore, this poster will also cover the recent advances in mechanochemical catalysis for plastic recycling, and present the possibility in coupling mechanochemistry with electrochemistry for valorising waste into green hydrogen and value-added chemicals.

Alternative Pathways for Sustainable Aviation Fuel Production from CO_2 and H_2: an Enviro-Economic Assessment *Andrea Bernardi (Imperial College London)*

The aviation industry is responsible for 2% of the total GHG emissions and 10% of the fuel consumption worldwide, with a predicted market growth of 3.7% a year. It is expected that a large portion of the current global fleet will continue to be operational until 2040-2050 calling for the development of drop-in alternatives based on sustainable resources.
Significant research efforts have been liquid fuels from CO_2 and H_2 leveraging the Fisher-Tropsch (FT) synthesis.

Continued ▶

However, the direct hydrogenation of CO_2 to liquid fuels in a single step is more appealing, but usually the formation of short chain hydrocarbons is favored. In this work, we carry out a techno-economic analysis and life-cycle assessment (LCA) of two SAF production processes: a one-step process (1sFT) based on the above-mentioned catalyst; and a two-step process (2sFT). 1sFT and 2sFT are simulated at scale using Aspen HYSYS to evaluate their economic performances and obtain inventories for the LCA. The environmental assessment is conducted in SIMAPRO 9.5, using Ecoinvent 3.9.1 Cut-Off database for the background process inventories. Our results show that the one-step process is superior both in economic and environmental terms to the two steps process, due to a lower capital cost, higher selectivity towards liquid hydrocarbons and lower energy requirements. On a well-to-wake basis the 1sFT process is predicted to reduce GHG emissions by 75% and the 2sFT process by 58%. The analysis of the endpoint environmental impacts confirms a better environmental performance of the synthetic fuels compared to the fossil counterpart, with the 1sFT outperforming the 2sFT by a larger extent, with 1sFT and 2sFT having a total externality cost 44% and 22% lower that the fossil fuel, respectively. At current CO_2 and H_2 prices the productions cost of low-carbon synthetic fuels is predicted to be 6-8 times higher than fossil-based aviation fuels, which agrees with the literature, and a combination of feedstock cost reduction and policy intervention (e.g. carbon taxation) is necessary for synthetic fuels to become cost competitive.

Optimising the Environmental Impacts and Process Efficiency in CO_2 Capture Technology through an AI-enabled Optimisation Framework
Xin Yee Tai (University of Surrey)

In the realm of carbon capture technology, specially using monoethanolamine (MEA) as the solvent, a well-established method involves separating CO_2 from industrial flue gas at the power plants. This process is marked by its high CO_2 reactivity and low production cost, allowing for large-scale and stable operation. Anticipating that higher MEA concentrations can enhance CO_2 capture rate, reducing energy consumption but potentially exacerbating environmental emissions due to an increased risk of corrosion and solvent degradation. Given the intricacies of the process, an imperative need arises for a resilient modelling and optimisation framework to effectively minimise energy consumption and environmental impact while maintaining high CO_2 capture efficiency. The study introduces a novel digital twin framework leveraging AI-enabled optimisation approach. This framework includes (1). a deep learning surrogate model for predicting the process metrics, (2). a life cycle assessment (LCA) to evaluate the environmental impacts, and (3). a NSGA-II (non-dominated sort genetic algorithm) algorithm for multi-objective

Continued ▶

optimisation. Initially, an ASPEN HYSYS model generates a database for a deep neural network (DNN), creating a surrogate model predicting energy demand, material consumption, and emissions. These predictions serve as input parameters for the subsequent LCA model, evaluating environmental impacts. Finally, NSGA-II is adopted to optimise CO2 capture efficiency and environmental impacts, identifying the trade-off between objective functions. AI-enabled optimisation proves promising for accurate prediction and effective optimisation, as demonstrated in our previous publications. Its robust computational capability can be utilised to systematically evaluate and optimise the multi-objective problem in MEA-based carbon capture.

Multi-scale Fuel Cell Electrode Design via Generative AI

Chongyuan Lu (Loughborough University)

The crucial advancement of hydrogen electrochemical energy devices requires the exceptional design of multi-scale electrode nanostructures. However, the complex interplay among multi-scale electrode components, high synthesis cost and vast design space have been formidable hurdles. Rational digital design tools play a key role in accelerating cost-effective design and optimisation of electrode nanostructures while remaining challenging so far. Here, we leverage the power of generative artificial intelligence (AI), multi-scale multi-physics modelling as well as physics-informed surrogate models to efficiently design and optimise electrode nanostructures of fuel cells, i.e., solid oxide fuel cell anodes and catalyst layers of proton exchange membrane fuel cells, driven by their ultimate electrochemical performance. The developed learning frameworks allow the inverse design of electrode nanostructures and enable the global optimisation of manufacturing parameters, e.g. Pt/C and I/C ratios for low Pt loading Pt-carbon-ionomer catalyst layers for proton exchange membrane fuel cells. The proposed deep learning frameworks are transferable to the design and optimisation of broad porous electrode nanostructures.

FACULTY OF ENGINEERING AND PHYSICAL SCIENCE

University of Surrey
Guildford, GU2 7XH, UK

surrey.ac.uk