Part I: Track Record

1. **The Principal Investigator**

I completed my PhD in 2014 at Newcastle University, where my research focused on modelling and experimental validation of electrochemical systems such as proton exchange membrane (PEM) fuel cells. Since then, I have held postdoctoral research positions at several universities, including the University of Birmingham, Purdue (USA), Oxford, Ulster, and Loughborough, before joining the University of Surrey as a Lecturer in Digital Chemical Engineering in 2022. I was the primary researcher in 8 research projects that were funded by EPSRC ([EP/G030995/1](https://gow.epsrc.ukri.org/NGBOViewGrant.aspx?GrantRef=EP/G030995/1), [EP/V042432/1](https://gow.epsrc.ukri.org/NGBOViewGrant.aspx?GrantRef=EP/V042432/1), [EP/V011863/1](https://gtr.ukri.org/projects?ref=EP%2FV011863%2F1)), Innovate UK (TS/L003473/1), NERC ([NE/P01982X/1](http://gotw.nerc.ac.uk/list_full.asp?pcode=NE%2FP01982X%2F1&cookieConsent=A)), EU H2020 FCH-JU ([875089](https://cordis.europa.eu/project/id/875089/reporting)) and NSFC (21878129, 21978118). I have published 1 book, 4 book chapters and several high-quality journal papers (including **4 ESI 1% Highly Cited Papers**) in highly visible journals, e.g., *AIChE J*, *Chem. Eng. Sci.*, *Chem. Eng. J.*, *Appl. Energy*, *Appl. Catalysis B* etc, with ***[h](https://scholar.google.co.uk/citations?user=mua8iv0AAAAJ&hl=en)*[-index](https://scholar.google.co.uk/citations?user=mua8iv0AAAAJ&hl=en)** of **28**. Additionally, I have filed 3 patents and delivered 2 invited/keynote presentations at international conferences, e.g., Newton Fund China-UK Research Links Workshop on Low- and Non-Pt Catalysts for PEM fuel cells in 2017 and the 6th [ICESCE](http://www.wikicfp.com/cfp/servlet/event.showcfp?eventid=107431&copyownerid=163220) in 2020, also 2 invited talks given at Illmenau University of Technology and Burapha University. I served as the **Vice President** of the UK Chapter of International Association for Green Energy (IAGE), with the main duties of promoting collaborations between green energy researchers in the UK and worldwide and the impact of the association. I was the **Technical Program Chair** of the 3rd [ICEAI](http://www.energy-ai.org/) i n 2022, that involved soliciting and evaluating conference papers and identifying the best papers to be published in Energy and AI. I have reviewed 30+ research proposals for funding bodies in the UK, China, and Hungary, as well as 100+ papers for leading journals such as *Adv. Funct. Mater.*, *Appl. Energy*, *Energy Convers. Manag* etc. I served as a Guest/Topic Editor for several special issues in high-impact journals, including *J. Energy Storage*, *Energies*, and *Front. Energy Res*. In addition, I am a **Chartered Member of IChemE** and an active member of several professional organisations, including ECS, ACS, and the [Alan Turing Institute’s Research and Innovation Cluster in Digital Twins](https://www.turing.ac.uk/research/harnessing-power-digital-twins/turing-research-and-innovation-cluster-digital-twins). Since 2021, I have been an associate member of the UKRI Interdisciplinary Centre for the Circular Chemical Economy (**CircularChem**), where I initiated circular economy research on promoting decarbonisation in industry. My research was primarily focused on the production of value-added chemicals through the recycling and reuse of CO2 emissions as feedstocks. My past research expertise, project experience and community service, coupled with my actively involvement in collaboration with academic and industrial partners in CircularChem, have provided me with valuable experience in working collaboratively in teams. My past research has demonstrated the effectiveness and feasibility of the multi-physics and data-driven modelling approaches on **CO2 capture and utilisation**. I strongly believe that the New Investigator Award presents a unique opportunity for me to take on a leadership role and conduct ground-breaking research that aligns with my long-term career objectives in the circular chemical economy, particularly circular fertiliser production system from the wastes in industry and agri-food.

1. **Recent Research Highlights**

My research interests revolve around the **multi-physics modelling** and **multi-objective optimisation** of **circular economy ecosystems** that involve interconnected chemical and electrochemical processes and devices, including fuel cells, waster electrolysers and CO2 capture and utilisation reactors powered by renewable energy. In the past few years, I have been focusing on using **machine learning (ML)** based **data-driven modelling** and **AI-aided decision-making** to expand the boundaries of traditional physics-based modelling approaches for dynamic optimisation of large-scale and complex models. As the lead researcher, I developed several multi-physics mechanistic and ML methods to address the multi-variable and multi-objective problems in the design and optimal control of CO2 capture reactors [[1](https://www.sciencedirect.com/science/article/pii/S1385894722054778),[2](https://www.sciencedirect.com/science/article/pii/S266654682300006X)] and functionally graded porous electrodes for PEM fuel cells [[3](https://www.sciencedirect.com/science/article/pii/S0009250922009356),[4](https://www.sciencedirect.com/science/article/pii/S0009250922006613?via%3Dihub)]. At Surrey, my research is focused on **AI-aided reinforcement learning** and **techno-economic analysis** (TEA) [[2](https://www.sciencedirect.com/science/article/pii/S266654682300006X),[5](https://www.sciencedirect.com/science/article/pii/S2352152X21001651?via%3Dihub)] of CO2 capture and utilisation system to underpin the Net Zero target of the UK. Preliminary studies of data-driven modelling [[1](https://www.sciencedirect.com/science/article/pii/S1385894722054778)] and TEA [[2](https://www.sciencedirect.com/science/article/pii/S266654682300006X)] have been published, which serves as the foundation for my proposed New Investigator Award project.

**(1) Experimental setup and evaluation of mass transport reinforced flow fields for electrochemical cells.** In PEM fuel cells, the gas diffusion electrode (GDE) under the rib area is susceptible to low local reactant concentration due to the low mass transfer rates caused by compression from the ribs. In response, I have developed innovative parallel flow fields with controllable adjacent channel pressure gradient [[6](https://aiche.onlinelibrary.wiley.com/doi/10.1002/aic.16957)] and auxiliary sub-channels and arrayed holes [[7](https://aiche.onlinelibrary.wiley.com/doi/10.1002/aic.17758),[8](https://aiche.onlinelibrary.wiley.com/doi/10.1002/aic.17461)] to enhance convective mass transport across the rib at a minimal pressure drop. In addition to multi-physics modelling, I employed cutting-edge manufacturing techniques, e.g., 3D metal printing, to fabricate these innovative flow fields and established experimental equipment to access their effectiveness. My research has demonstrated that these two novel flow fields improved cell performance by 40% and 25% with a minimal pressure drop lower than 100 Pa at 0.4 V, respectively. The practical experience I have obtained from fabricating and testing electrochemical devices can be utilised in designing the urea electrosynthesis hardware (**WP1**) proposed for this project.

**(2) Multi-objective process optimisation of CO2 capture reactors based on multi-physics and data-driven modelling.** I applied the multi-physics, machine learning (ML), multi-variable, and multi-objective simulation approach on enhanced weathering (EW) based CO2 capture reactor design and optimisation [[1](https://www.sciencedirect.com/science/article/pii/S1385894722054778),[2](https://www.sciencedirect.com/science/article/pii/S266654682300006X),[9](https://www.sciencedirect.com/science/article/pii/S1385894721056709?via%3Dihub)]. An important result of our study is the development of a data-driven model called extended adaptive hybrid functions (E-AHF) [[1](https://www.sciencedirect.com/science/article/pii/S1385894722054778),[2](https://www.sciencedirect.com/science/article/pii/S266654682300006X)], which combines the strengths of five individual surrogate models ([RSM](https://en.wikipedia.org/wiki/Response_surface_methodology), [Kriging](https://en.wikipedia.org/wiki/Kriging), [RBF](https://en.wikipedia.org/wiki/Radial_basis_function), [SVM](https://en.wikipedia.org/wiki/Support_vector_machine) and [MLS](https://en.wikipedia.org/wiki/Moving_least_squares" \l ":~:text=Moving%20least%20squares%20is%20a,the%20reconstructed%20value%20is%20requested.)) to enhance the prediction accuracy for packed bubble column (PBC) reactors with 8 design variables. My current work focuses on optimising the multi-objective predictive optimisation of an EW-based CO2 capture process in response to intermittent flue gas and renewable energy supply. I used an advanced ML algorithm ([LSTM + Lagged feature](https://machinelearningmastery.com/reshape-input-data-long-short-term-memory-networks-keras/)s) to predict CO2 emissions and renewable energy, and proposed an adaptive optimisation framework for the flexible operation of EW-based PBC in response to fluctuations in CO2-rich flue gas. The experience in developing complex physics-based model, data-driven model and ML approaches can be directly implemented in **WP2** of my proposed research.

**(3) Techno-economic analysis (TEA) of hydrogen-based energy storage system (ESS) and CO2 capture process in a circular economy system.** I supervised a PhD student to conduct a TEA for a ESS using hydrogen via water electrolysis as an energy carrier to mitigate the variability of renewable sources, based on the meteorological data from two case-study locations [[5](https://www.sciencedirect.com/science/article/pii/S2352152X21001651?via%3Dihub)]. It was found that the hydrogen-based EES had a more favourable levelised energy cost of 227 and 167 $/MWh for the respective locations compared to a traditional battery storage system. Additionally, the TEA for enhanced weathering based CO2 capture revealed a net cost of approximately 400 $ per ton of captured CO2, which is 25% lower than current direct air capture (DAC) technologies [[2](https://www.sciencedirect.com/science/article/pii/S266654682300006X)]. This knowledge and practice in TEA could be applied directly to **WP3** of the proposed project.

1. **Research Environment**

The University of Surrey is a leading research-oriented institution. According to the Guardian University Guide 2023, Surrey is ranked 24th in the UK, while the latest REF2021 places Surrey at 15th in the UK for research power in engineering. The university has established two pan-University institutes, namely the **[Surrey Institute for People-Centred AI](https://www.surrey.ac.uk/artificial-intelligence)** and the **[Institute of Sustainability](https://www.surrey.ac.uk/institute-sustainability)**. I am a Fellow of both institutes, actively participating in various initiatives, such as co-supervising an AI-based MSc programme and collaborating on life cycle assessment (LCA) research. **Energy** and **Circular Economy** are key research focuses of the School of Chemistry and Chemical Engineering, with more than 20 academic staff with strong modelling skills and experience. The School have provided me a start-up package, including a PhD studentship (**starting in Sep. 2023**), a high-performance workstation and reduced teaching load. I am a member of the information and process systems engineering ([IPSE](https://www.surrey.ac.uk/school-chemistry-and-chemical-engineering/research/information-and-process-systems-engineering)) team, which provides me with access to a small high-performance cluster that is capable of handling complex tasks related to modelling and machine learning.

1. **Collaborators and Partners**

Based on our shared interest in circular chemical economy, I have formed partnerships with renowned researchers in the field (see letters of support). My industrial partner **OxCCU** will supply the state-of-the-art catalysts for the fabrication of GDE-based urea electrosynthesis electrolyser (**WP1**). **Siemens PSE** and **Intelligent Plant** will work closely with us to implement the research outcomes (**WP2** and **WP3**) in their digital products, e.g., gPROMS and applications hosted in their Industrial App Store. **CircularChem** will offer both technical assistance and consulting services throughout the project, including support in the development of electrochemical devices and systems, as well as the provision of CO2 pricing data. **[Prof. I.A. Ieropoulos](https://www.southampton.ac.uk/people/5z9k7x/professor-yannis-ieropoulos)** at Southampton will collaborate in the project by offering technical assistance in hardware design and assembly (**WP1**). **[Dr. L. Lu](https://directory.seas.upenn.edu/lu-lu/)**, my established collaborator at UPenn, will co-supervise PhD students for developing PINN models (**WP2**). **[Prof. J. Sadhukhan](https://www.surrey.ac.uk/people/jhuma-sadhukhan)** at Surrey will assist circular economy and sustainability (**WP3**). The collaboration will help them expand impact and find potential partners in CircularChem community.

Part II: Case for Support

1. **Project vision, aim and innovation**

My **vision** is to develop a **circular fertiliser production system** across the UK industry and agri-food sector that will help achieve the Net Zero 2050 target. The **aim** of the project is to develop an novel **electrochemical urea synthesis** with **carbon utilisation** (EUS-CU) process, and integrate the process into the wider industrial and agri-food nexus, in which emitted nitrogenous wastewater and CO2 can be simultaneously converted to urea – a nitrogen-containing fertiliser.

The vision is underpinned by the following set of key scientific innovations:

1. Development of a prototype for the EUS-CU process based on gas diffusion electrodes (GDEs) and microfluidic configuration operated at continuous condition, that is incorporated in a hardware-in-the-loop platform with automation functionality (**WP1**).
2. Construction of an interpretable digital twin for the EUS-CU process to enable self-optimisation in response to multiple objectives and constrains, e.g., conversion, product yield, intermittency of renewable energy and product demand (**WP2**).
3. Integration of the EUS-CU process into a circular economy ecosystem and creation of a multi-criteria assessment framework through a whole-system approach (**WP3**).

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描述已自动生成Establishing a circular economy in UK’s industry and agri-food sectors for sustainable urea production is a viable approach towards Net Zero. This is because the chemical industry in the UK is the second largest industrial emitter, and the agriculture also produces significant greenhouse gas (GHG), e.g., nitrous oxide, methane, and CO2, which are difficult to recycle and reuse. The fertiliser, steel, and metal industries (e.g., CF industries and British Steel in Teesside industrial cluster) are the primary sources of nitrogenous wastewater, with nitrate concentration ranging from 600 to 1000 mg/L. Furthermore, the UK has a plentiful supply of wind energy that could be utilised as a substitute for fossil fuel-based energy sources, e.g., Dogger Bank wind farm located at the Northeast coast of England could provide annually 3.6 GW electricity. To achieve sustainable manufacturing with resource resilience and economic viability in the future, it will be crucial to implement circular economy systems throughout the entire lifecycle of urea production. By incorporating the EUS-CU process into industry and agri-food, a circular economy ecosystem can be established to manage nitrogenous wastewater and CO2 emissions (Fig. 1). The novelty of the circular economy urea production system lies in its ability to reuse waste and pollution by closing the loop on resources. The digitalisation of the system provides real-time monitoring and optimal control of the production process in response to dynamic variation of resources and energy, which enables better decision-making by improving system efficiency and minimising environmental impact.

1. **State-of-the-art**

**Scientific challenge**: Urea is a widely used nitrogen-based fertiliser that has traditionally been produced through an energy-intensive Haber-Bosch process and results in large amounts of CO2 emission, which accounts for 2% of the global energy consumption and 1% of annual anthropogenic greenhouse gas (GHG) emissions [[10](https://www.frontiersin.org/articles/10.3389/fenrg.2021.580808/full)], which is not compatible with the Net Zero 2050 target set by the UK government to combat climate change. Meanwhile, the significant quantities of wastewater and GHG emissions in industry and agri-food open new opportunities to utilise these waste products to achieve sustainable urea production and prevent environmental pollution. Hence, a promising approach for synthesising urea while utilising carbon dioxide is a single-step **electrochemical urea synthesis** with **carbon utilisation** (**EUS-CU**). This approach has great potential, particularly for UK’s chemical industrial, where abundant nitrogenous and carbon waste are generated. To date, approximately 9.3 kg/day of urea production (based on 100 g of catalyst with a maximum urea yield rate of 64.76 mmol g-1 cat h-1) has been achieved using the state-of-the-art electrochemical catalyst [[11](https://pubs.acs.org/doi/10.1021/acsnano.2c11046?ref=PDF)]. Nevertheless, there has been a lack of research attention to urea electrosynthesis process and system design. In particular, the integration of EUS-CU into industry and agri-food sectors and the digitalisation of the constructed circular economy ecosystem are unexplored fields.

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描述已自动生成**Research gap 1**: Using nitrite (NO-2)/nitrate (NO- 3) wastewater as nitrogen sources for urea electrosynthesis is a more practical option than N2 due to its low dissociation energy (~200 kJ mol-1 vs. 941 kJ mol-1 for N2 gas) and superior solubility in water. The highest recorded urea yield rates to date are 64.76 and 29.97 mmol g-1 cat h-1 for the NO-2-CO2 and NO- 3-CO2 systems, much higher than the urea yield rate based on N2 gas (14.5 mmol g-1 cat h-1) [[12](https://pubs.rsc.org/en/content/articlelanding/2022/ee/d1ee03918k),[13](https://www.sciencedirect.com/science/article/pii/S2666386422001436),[14](https://onlinelibrary.wiley.com/doi/full/10.1002/aenm.202201500)], and the maximum faraday efficiency for the two systems is 43.1% [[15](https://www.sciencedirect.com/science/article/pii/S0021979720306081)] and 69.1% [[16](https://pubs.rsc.org/en/content/articlehtml/2023/ey/d2ey00038e)], respectively**. However, most laboratory-scale electrolysers are not suitable for upscaling the process** due to the use of H-type design, which involves separating the anode and cathode electrolytes with a membrane, merging the catalyst-coated plate into the nitrogenous solution, and introducing CO2 through bubbling. While this design is appropriate for studying the reaction kinetics at low current densities, where mass transport is not a significant factor, it is not suitable for continuous industrial urea production due to small specific area and high mass transport resistance. The practical application of urea electrosynthesis requires large electrode surface area, e.g., a few hundred cm2, lead ing to a more significant mass transport influence. **A microfluidic electrolyser based on gas diffusion electrodes (GDEs)** (Fig. 2) would be a more suitable option to create a controllable operational environment that closely resembles real-world industrial applications [[17](https://www.sciencedirect.com/science/article/pii/S2212982018310217)]. However, no research has been conducted on the development of electrolyser units for continuous urea electrosynthesis in industrially relevant conditions that can be replicated using hardware-in-the-loop. This will be addressed in WP1.

**Research gap 2**: To optimise the EUS-CU process within a circular economy system, it is essential to have a thorough understanding of the underlying physicochemical interactions that occur within the electrochemical unit, as well as the complex dynamics that arise when integrating this unit into the broader manufacturing process. To achieve a prompt response in system-scale modelling while considering the influence of various operating parameters on multiple processes within the system, it is critical to implement the **digital twin approach**, in which the **physics-based models** for each individual process is substituted with **data-driven surrogate models**. To create sophisticated physics-based models of the EUS-CU process, it is important to identify the values of key parameters that respond to different electrochemical activities and selectivity of diverse catalysts. Due to the diverse reaction elementary steps and kinetics parameters in different catalytic systems, e.g., PdCu [[16](https://pubs.rsc.org/en/content/articlehtml/2023/ey/d2ey00038e)], Fe-Ni [[18](https://www.nature.com/articles/s41467-022-33066-6)], Vo-CeO2 [[19](https://pubs.acs.org/doi/full/10.1021/jacs.2c03452)], it is a big challenge to accurately simulate the EUS-CU process with respect to different catalysts and operating conditions. Based on published data, machine learning algorithms [[20](https://www.frontiersin.org/articles/10.3389/fenrg.2021.609070/full)], e.g., XGBoost, CatBoost, AdaBoost, can be used to determine these key parameters according to statistic principles that may not be apparent with traditional experimental methods. This allows for efficient determination of the values of key kinetic parameters under various operating conditions and catalyst environments, which will be incorporated into the physics-based models. To achieve multi-level materials and energy flow optimisation for integrated continuous urea electrosynthesis process in complex circular economy systems, a digital twin of the EUS-CU unit can be developed and integrated. However, the challenge in creating a digital twin lies in efficiently linking it with the physical process, in which the real-time changes can be accurately reflected in the digital twin. **The innovation lies in the creation of interpretable machine learning (ML) models**, e.g., physics-informed neural network (PINN), which will **not only significantly improve the accuracy of the ML models but also increase their ability to be applied to new scenarios and maintain their performance while requiring less training data**. By coupling the interpretable digital twin with cutting-edge optimisation algorithms, the EUS-CU process can be optimised in response to fluctuations in renewable energy, nitrogen and carbon resources while considering multiple objectives and constrains. This will be addressed in WP2.

**Research gap 3**: The intermittent supply of nitrogenous wastewater, CO2, and renewable energy in industry and agri-food, along with fluctuations in market demand for urea products, necessitates dynamic and adaptive optimisation strategies that can respond to real-time supply conditions. To ensure the maximum product yield at the highest process efficiency and at the lowest energy consumption, it is crucial to optimise the circular economy ecosystem at a higher level based on predictions of the next-hour availability of reactants and energy using state-of-the-art AI algorithms and historical data. This underpins the importance of implementing a dynamic system-level optimisation approach that can adapt to changing conditions and ensure balanced resource allocation. The predictions of environmental parameters, e.g., renewable energy, waste emissions, and the urea market demand, can be served as input variables in the process-scale digital twin developed in WP2. Then, a techno-economic analysis (TEA) and life-cycle assessment (LCA) can be performed to evaluate the economic and circularity (e.g., wastes reuse efficiency) of the proposed urea electrosynthesis process within a circular economy ecosystem. This approach will create unique digital intelligence that informs multi-criteria assessment and optimisation strategies by exploring the underlying mechanism of urea electrosynthesis process, rather than a ‘data fitting’. **The proposed multi-criteria assessment framework (MCAF) is innovative as it incorporates in-silico EUS-CU performance and digital-twin information, economic and environmental impact data.** The tool based on MCAF will provide a scientific assessment of the sustainability of the proposed system and generate recommendations for future policy making based on real-time 图示

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In essence, the project’s transformational nature is centred on creating the first circular urea production economy system at the intersection of industry and agri-food. This will involve developing a ground-breaking hardware-in-the-loop platform for the urea electrosynthesis unit (WP1), which will be connected to a beyond-current-state-of-the-art digital twin of the manufacturing process (WP2), dynamically optimised by AI-aided adaptive optimisation algorithm on real-time environmental conditions and guided by system-level sustainability and circularity assessment (WP3). The three WPs will be interactive, with continuous flow exchange of real-time data and knowledge (Fig. 3).

1. **Research programme**

Our proposed research consists of three interconnected work packages (WPs), including hardware design, digital twin creation, and multi-criteria assessment of system circularity and sustainability. We begin with a creation of a hardware-in-the-loop platform with automation functionality that integrates EUS-CU reactor prototype and real-time simulator, in which the fluctuations of environmental variables could be simulated and fed into the platform as input variables. We will also develop a digital twin for the EUS-CU process to achieve rapid optimisation of the EUS-CU process in response to environmental variables. Techno-economic analysis (TEA) will be conducted to evaluate the circularity and sustainability. Detailed tasks of the three WPs are given as follow:

**WP1. EUS-CU process hardware-in-the-loop and automation platform (PI and PhD students).**

We will create a hardware-in-the-loop platform to test a EUS-CU single-cell unit in a controllable environment that represents the characteristic of industry and agri-food sectors (Fig. 4).

Task 1.1. Fabrication of continuous microfluidic electrolyser prototype. The gas diffusion electrode (GDE)-based microfluidic electrolysis prototype, with a transparent window opened on the bipolar plate, for urea electrosynthesis prototype (50-100 cm2 surface area) using continuous-flow CO2 and nitrogenous wastewater as N source will be developed (**Task 1.1a**). Different electrochemical catalysts provided by industrial partner or prepared in-house, e.g., the Cu2O/graphene previously prepared [[21](https://www.sciencedirect.com/science/article/pii/S0926337321011474)], will be prepared as catalyst ink and sprayed onto carbon paper to prepare the GDE. Instead of H-type electrolyser in lab-scale, a single-cell microfluidic electrolyser will be fabricated by hot-pressing the as-prepared GDE with proton exchange membrane and bipolar plates of 50-100 cm2 electrode area. To reinforce the mass transport of nitrogenous wastewater and CO2 through the GDE, we will introduce some new flow fields to the electrolysers, including the convection-enhanced serpentine flow field [[22](https://www.sciencedirect.com/science/article/pii/S019689042300211X)] and Tesla valve flow field [[23](https://www.sciencedirect.com/science/article/pii/S0306261922015331)], and compare their performance to that of the traditional parallel flow field. Additionally, we will assess the effect of different flow field configurations in relation to the size of the electrolyser, which will aid us in understanding the mechanisms of electrolyser’s surface area on the electrochemical performance, i.e., conversion rate, efficiency, and product yield (**Task 1.1b**). This physical prototype will serve as a platform for gathering data to validate the physics-based models developed in **WP2**.

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Task 1.2. In-situ and in-operando characterisation of the electrolyser prototype. We will develop an instrumented system that can imitate the thermohydraulic-electrochemical dynamics observed in production-scale environments. The electrolyser prototype developed in **Task 1.1** will be integrated with different microscopic techniques, including high-speed cameras, thermal couples, and humidity sensors, to map the distributions of crucial internal states such as flow field, temperature and relative humidity profiles under varying design and operating conditions. [Liquid chromatography–mass spectrometry](https://en.wikipedia.org/wiki/Liquid_chromatography%E2%80%93mass_spectrometry) (LCMS) will also be incorporated to dynamically measure the production composition. Thus, sufficient data for a variety of operating conditions, electrode properties and flow filed configurations can be obtained to validate the physics-based model developed in **WP2**.

Task 1.3. Automation of the hardware-in-the-loop (HIL) platform. We will create a HIL platform that can replicate changes in input parameters for an electrolyser operated under industrial conditions, such as intermittent wastes and wind energy. The entire platform comprises workstation, data acquisition hardware (e.g., thermal couples, pressure sensors, humidity sensors, high-accuracy flow meters and large measurement equipment in **Task 1.2**), simulation software (LabView, Simulink etc.), EUS-CU electrolyser, and the associated control system. The environmental parameters, e.g., the fluctuations of nitrogenous wastewater, CO2, urea demand and wind energy, will be simulated and used as input variables of the HIL platform. The output parameters include product composition, product yield, current density etc. Then the platform will be equipped with automated experimentation capabilities to allow for autonomous adjustments of process variables like reactant concentrations, flow rate and power input. The *plug and play* programmable automation system is customised and controlled by LabView or MATLAB. The HIL platform will enable high-throughput data generation from online monitoring, which will be transmitted to the data-driven surrogate model, creating possibilities for AI algorithms developed in **WP2** to facilitate autonomous optimisations.

**WP2. Physics-based models and interpretable digital twin of EUS-CU process (PI and PDRA).**

We will develop physics-based models for the EUS-CU process that will produce data (in conjunction with experimental data) for training data-driven surrogate models. Optimisation algorithms will be integrated into the surrogate models to determine the optimal operation condition.

Task 2.1. Development of sophisticated physics-based mechanistic models. The development of time-dependent, non-isothermal, multiphase flow, physics-based EUS-CU models enables the coupling of reaction kinetics, mass transport, fluid dynamics and conservation of energy. Thus, it permits a thorough comprehension of how different variables from diverse physical and electrochemical processes interact with each other, going beyond the traditional approach of relying solely on experimental trial-and-error. These physics-based models are designed using 3D geometry, with varying electrode surface area and flow field configurations to enable the numerical investigation of time-dependent response of multiple variables (reactant concentration, flow rate, cell voltages etc) on multiple objectives (conversion, faraday efficiency, product yield etc). The physics-based models will be rigorously validated through experimental measurements in **WP1**, e.g., the predicted polarisation curves, faraday efficiency and conversion under various operating conditions are validated by experimental data to guarantee the accuracy and reliability of the physics-based models.

Task 2.2. Determination of key kinetics parameters using cutting-edge AI. It is a great challenge to determine the values of various key parameters, e.g., charger transfer coefficient, exchange current density and equilibrium overpotential, for a range of catalysts and reaction routes that are included in the EUS-CU process. To overcome this challenge, available published data can be used to train AI models, e.g., recurrent neural network (RNN) [[3](https://www.sciencedirect.com/science/article/pii/S0009250922009356)], which can learn to recognise patterns and trends in the data and use this information to predict the values of key parameter for different catalysts and reaction conditions. We will also generate new data with the prototype developed in **WP1** to enrich the database for AI model training.

Task 2.3. Interpretable digital twin of EUS-CU process and multi-level optimisation. The goal of this task is to create a reliable digital twin that significantly reduces computational time. The digital twin will be developed by coupling the EUS-CU hardware (in **WP1**) with the data-driven surrogate models based on machine learning (ML) approaches, which is trained by the data produced by both experimental measurement (**Task 1.2**) and multi-physics simulation (**Task 2.1**). We will evaluate various ML approaches, e.g., SVR, ANN, E-AHF [[1](https://www.sciencedirect.com/science/article/pii/S1385894722054778),[2](https://www.sciencedirect.com/science/article/pii/S266654682300006X)], to effectively construct a reliable connection between key design parameters of electrolyser properties (e.g., catalyst loading, porosity, surface area) and operating conditions (e.g., CO2 partial pressure, wastewater flow rate) and objective functions (e.g., conversion, product yield). We will also exploit state-of-the-art ML approaches, for example, integrating physical knowledge (e.g., partial differential equations, symmetries, conservation laws) into the ML model to build physics-informed neural networks (PINNs). This will not only substantially enhance the precision of the ML models, but also increase their generalisability and stability, while reducing the need for training data. In addition to mature [GA](https://en.wikipedia.org/wiki/Genetic_algorithm), [NSGAII](https://en.wikipedia.org/wiki/Multi-objective_optimization) optimisation algorithms, we will try novel optimisation methodologies e.g., Harris Hawks algorithm [[24](https://www.sciencedirect.com/science/article/pii/S0167739X18313530)] and Grey Wolf Optimiser [[25](https://www.sciencedirect.com/science/article/pii/S0965997813001853)], to achieve the optimal design parameters and operating conditions of the reactor at steady-state operating conditions. We will find the most effective experiment-validated data-driven models to create an opensource software/applications to be hosted on industrial partner’s website and Industrial App Store. Users can customise the values of multiple design variables and obtain electrolyser performance indicators (e.g., product yield, conversion, energy consumption etc.) through cloud computing, and the optimal design variables will be automatically calculated.

**WP3. AI-aided system dynamic optimisation and multi-criteria assessment (PI and PDRA).**

We will embed the interpretable data-driven models of EUS-CU process (in **WP2**) into a circular economy ecosystem and enable the system with adaptive optimisation functionality in response to fluctuated environment parameters with AI. We will also establish a multi-criteria assessment framework (MCAF) to evaluate the circularity and sustainability of the EUS-CU based ecosystem.

Task 3.1. Prediction of waste resources and renewable energy.We will collect data on nitrogenous wastewater discharge, CO2 emission, and electricity generated from renewable energy in a real UK industrial cluster (e.g., wind in Teesside) from available database, e.g., [CEDA Archive](https://archive.ceda.ac.uk/), or contacting the primary emitters for required historic data. We will then implement advanced ML algorithms, e.g., long short-term memory network (LSTM) and two-stage multilayer perceptron network (MLP), to predict the next-hour availability of resources and energy.This will lay the foundation for the subsequent system-level adaptive optimisation.

Task 3.2. Reinforcement leaning based system-level dynamic optimisation. The surrogate models of the EUS-CU process developed in **Task 2.3** will be integrated into a circular economy ecosystem, in which the electrochemical processes are affected by numerous factors from the industry and agri-food (e.g., periodic waste material emission as feedstock, intermittent renewable energy, real time product demand) and the conversion device itself (performance degradation and efficiency reduction). We will tailor a multi-domain digital process framework to enable the prediction of the EUS-CU processes within the whole system in response to the intermittent supply of resources and energy, followed by a system-level dynamic optimisation powered by reinforcement learning (RL). RL enables the hardware (electrosynthesis reactor) in **Task 1.1** to learn through interactions with its surrounding environment by receiving feedback in the form of rewards and penalties that helps the hardware to determine the most appropriate actions to achieve a particular objective, e.g., lowest energy consumption, highest product yield etc.

图示

描述已自动生成Task 3.3. System circularity and sustainability evaluation through multi-criteria assessment framework.We will develop a multi-criteria assessment framework (MCAF), in which the dynamic operational influencing factors identified in **Task 3.2** are controlled that allows predictable dynamic adjusting and planning (see Fig. 5). A techno-economic analysis (TEA) model [[5](https://www.sciencedirect.com/science/article/pii/S2352152X21001651?via%3Dihub)] will serve as a springboard and produce essential references for understanding the economic and environmental impacts from integrating the EUS-CU process into a system. Carbon pricing will be considered in the TEA model to demonstrate the economic benefits of adopting the circular urea production process instead of the conventional linear process. The TEA model will use hourly waste emissions and meteorological data, e.g., temperature and wind speed, along with capital costs and real-time carbon price (e.g., [carbon price tracker](https://ember-climate.org/data/data-tools/carbon-price-viewer/)), to determine the cost of urea production for the circular economy ecosystem. Waste reuse efficiency will be used to evaluate the system circularity. Considering the project length, the system sustainability will be simply evaluated through carbon footprint analysis [[26](https://www.nature.com/articles/s43016-023-00698-w" \l "Sec13), [27](https://www.fertilizerseurope.com/wp-content/uploads/2020/01/The-carbon-footprint-of-fertilizer-production_Regional-reference-values.pdf)], in which the reduced CO2 emission is calculated. We will also conduct preliminary LCA study if time allows. The MCAF will offer decision-makers with scientific evidence to understand the circularity and sustainability of the circular urea production ecosystem.

1. **National importance**

The project aims to address the UK’s need for sustainable manufacturing and industrial decarbonation, which are critical for the country’s economic success. Developing digitalised and automated manufacturing processes is vital to maintain the UK’s competitiveness in the global market, and it can help maximise resource utilisation and reduce greenhouse gas emissions. Urea production is essential for agri-food in the UK and beyond, and sustainable urea production can provide food security, environmental benefits, and economic advantages by creating jobs, promoting innovation, and attracting investment. This research project will establish a world-leading activity that combines electrosynthesis and carbon utilisation to address sustainability challenges. The proposal aligns with EPSRC research themes, including Manufacturing the Future, Manufacturing Made Smarter, Circular Economy, and Industrial Decarbonisation, and it will establish the scientific and technical principles needed to develop a sustainable economy in the UK.

1. **Project management**

I will lead the project with limited assistance from a small advisory panel consisting of two knowledgeable academic staffs, [Prof. Jin Xuan](https://www.surrey.ac.uk/people/jin-xuan), and [Prof. Adrian Dobbs](https://www.surrey.ac.uk/people/adrian-dobbs). They will offer guidance on managing the team and acquiring resources, and we will hold quarterly meetings to track the project’s progress. Additionally, they will help to assemble a panel for a mid-term review. To keep the team on track, I will schedule weekly meetings to discuss any technical or operational issues and risks. I will also create an online group and a shared folder in MS Teams for sharing documents and having ad-hoc discussions. To address the risks associated with recruitment, I will use flexible start dates for PDRA and promote the project through our current research network, e.g., CircularChem and [Alan Turing Institute’s Research and Innovation Cluster in Digital Twins](https://www.turing.ac.uk/research/harnessing-power-digital-twins/turing-research-and-innovation-cluster-digital-twins). The detailed **key risks** and their **mitigation actions** of each WP can be found in the **workplan**. I will embed **EDI** during the planning of all activities, e.g., recruitment, research, discussion, networking, dissemination, and management of the project. I will also support the PDRA and PhD to achieve their career goals through the bespoke training programmes provided by the Doctoral College at Surrey.

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