CAMBRIDGE **CARES**

A RESEARCH COLLABORATION PLATFORM: UNIVERSITY OF CAMBRIDGE AND SINGAPORE

Biannual Research Report
October 2024 - March 2025

CAMBRIDGE CARES

CAMBRIDGE CENTRE FOR ADVANCED RESEARCH AND EDUCATION IN SINGAPORE LTD

Cover image

The picture shows the Chairman of NRF and the former Deputy Prime Minister of Singapore (2019–2025), Mr Heng Sweet Keat, in the leftmost position visiting CARES in December 2024 to learn more about the two CARES projects under the new SGD$90m Decarbonisation programme funded by the National Research Foundation.

The two CARES projects are HYCOMBS (page 49) and SM_3 (page 53).

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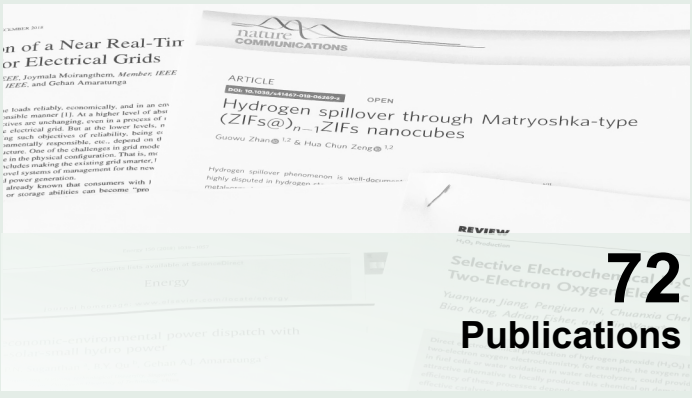

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FOREWORD

CARES has introduced a new management structure from the start of 1st January 2025 since the departure of our Founding Director (2013–2024), Prof Markus Kraft. The new structure consists of four Directors and Ms Elizabeth MacRae as the Chief Operating Officer.

- Prof Dame Lynn Gladden (Director of Research and Strategy)
- Prof Alexei Lapkin (Director of Entrepreneurship)
- Prof Epaminondas Mastorakos (Director of Industrial Relations)
- Prof Henriëtte Hendriks (Director of Education and Skills)

Prof Gladden has a longstanding connection with CARES, having been Pro-Vice-Chancellor for Research at the University of Cambridge (2010–2016) and playing a key role in the centre's founding. Prof Lapkin, Prof Mastorakos, and Prof Hendriks are all leading CARES research programmes, these are SM_3, HYCOMBS, and CLIC respectively.

The new structure will provide a fair representation of CARES across our decarbonisation and human health-related projects for the Singapore research landscape. The Chief Operating Officer, based fully in Singapore, will ensure that day-to-day activities run smoothly.

Deputy Prime Minister's visit December 2024

CARES recently welcomed Mr Heng Swee Keat, the Chairman of NRF and the former Deputy Prime Minister of Singapore (2019–2025) to our centre. The visit provided valuable time for our programme leads in the new decarbonisation projects (SM_3 and HYCOMBS) to explain the technical areas we aim to develop in Singapore: transport, energy, and manufacturing. The CARES lab tour provided an opportunity for our team to share the equipment that will be used in our projects and the local talent involved. The visit presented an incredible opportunity to speak openly with key decision-makers in the Singapore research landscape.

Strengthening Cambridge connections

CARES welcomed two visits in March 2025. The first was a knowledge exchange with the central Cambridge Communications team, focused on addressing knowledge gaps and providing a first-hand view of the impact of CARES' research in Singapore. The second visit marked Gates Cambridge's first trip to Singapore for their 25th anniversary, involving a lunch reception for Gates Scholars and running scholarship interviews in the CREATE building, featuring several CARES Professors as panellists. In May 2025, CARES collaborated with Cambridge Admissions to organise a postgraduate offer holder event, with contributions from CARES alumni and Prof Henriëtte Hendriks as speakers.

CLIC moves to the CREATE building

CLIC recently completed the arduous process of moving its main base from Nanyang Technological University. The closer proximity to CREATE has already created more visibility, such as speaking opportunities with other CREATE entities, involvement with high-profile visits, and stronger interactions with other CARES programme members.

We hope you have enjoyed reading the last half-year of highlights from CARES. Please get in touch with us if you would like to know more about our work or have ideas for collaboration.

ABOUT US

Cambridge CARES is the University of Cambridge's presence in Singapore

The Cambridge Centre for Advanced Research and Education in Singapore (CARES) is a wholly-owned subsidiary of the University of Cambridge. Cambridge CARES is funded by the National Research Foundation (NRF) as part of CREATE (Campus for Research Excellence and Technological Enterprise). We have a number of research collaborations between the University of Cambridge, Nanyang Technological University, the National University of Singapore, industrial partners, and other universities in Japan, France, Norway, and Switzerland.

The first programme administered by CARES is the Cambridge Centre for Carbon Reduction in Chemical Technology (C4T). The C4T programme is a world-leading partnership between Cambridge and Singapore, set up to tackle the environmentally relevant and complex problem of assessing and reducing the carbon footprint of the integrated petro-chemical plants on Singapore's Jurong Island. It brings together researchers from chemical engineering, biotechnology, chemistry, biochemistry, information engineering, electrical engineering, materials science, and metallurgy.

The motivation for the C4T project is to provide a rich pipeline of scientific insight and technological innovation with high potential for positive results within the decarbonisation agenda if deployed by appropriate industry and government parties. The split work streams within C4T has evolved to the now titled CNs that combine state-of-the-art experimental analysis with advanced modelling research from Cambridge and Singapore. Each CN has clearly defined milestones and deliverables with significant interaction between projects.

The first five-year research phase of C4T came to an end in October 2018. The programme received a further five years of funding for Phase 2, which commenced in November 2018 and has recently been further extended to 2025.

A second large CREATE-funded programme, the Centre for Lifelong Learning and Individualised Cognition (CLIC), began in October 2020. CLIC is a collaboration between the University of Cambridge and NTU and focuses on the neuroscience of learning, a new research area for CARES. CLIC has received confirmation of a further three years of funding, extending the programme to September 2026.

CARES is hosting two new projects under the SGD$90m Decarbonisation programme

announced by NRF in July 2024. These are Hydrogen and Ammonia Combustion in Singapore (HYCOMBS), and Sustainable Manufacture of Molecules and Materials in Singapore (SM_3). New collaborators on these projects include Tohoku University, CNRS, the Norwegian University of Science and Technology, and the Swiss Federal Technology Institute of Lausanne.

The Health-driven design for cities (HD_4) programme has also been included in this reporting period. HD_4 will investigate the relationships of the built environment on resident's behaviour and health outcomes.

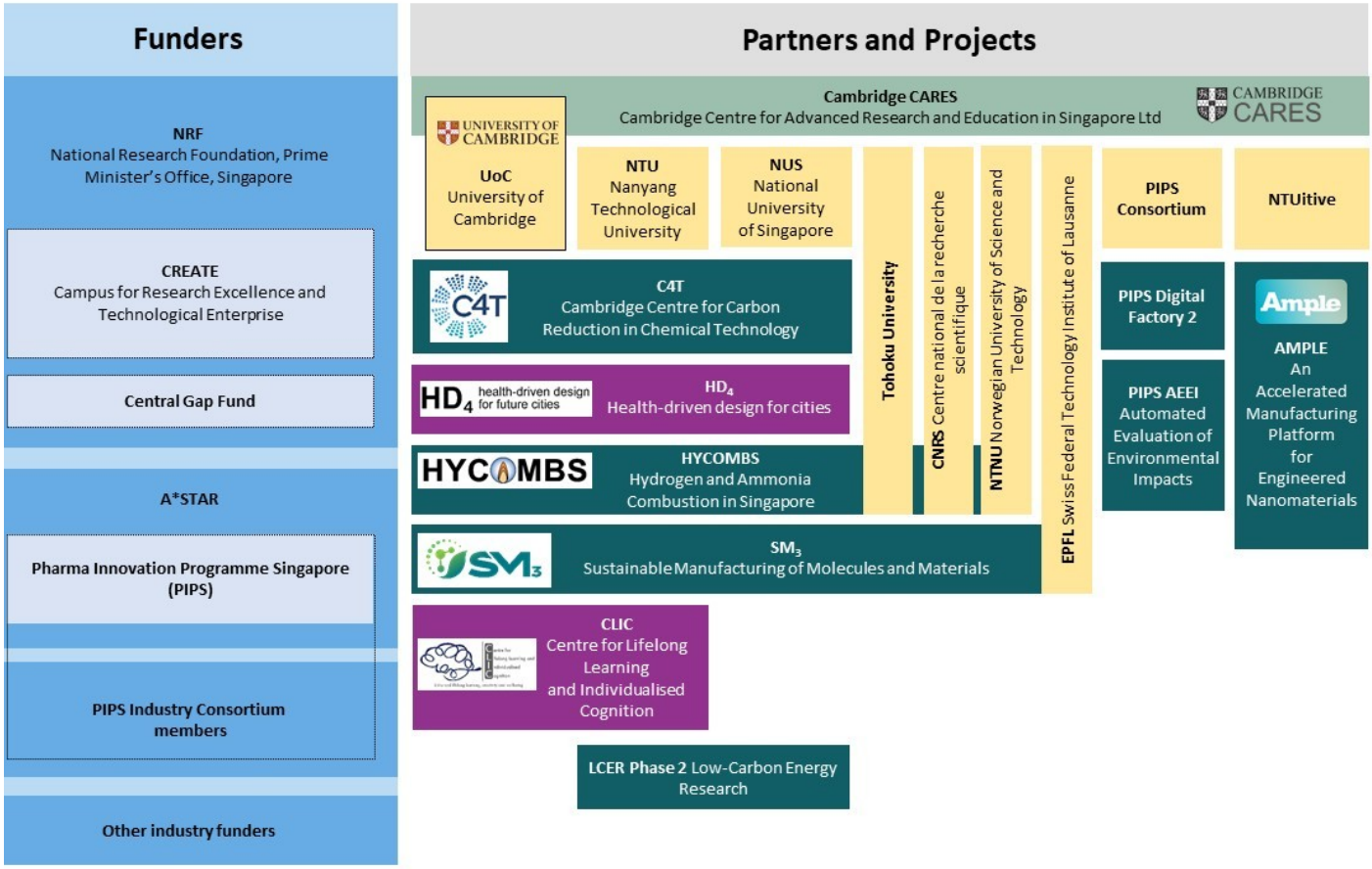
CARES is also hosting AMPLE (An Accelerated Manufacturing Platform for Engineered Nanomaterials), funded by the Central Gap Fund. AMPLE grew from research within the C4T programme and is currently looking to bring their products to commercialisation via the spin-off company Accelerated Materials.

There are currently two ongoing streams under the Pharmaceutical Innovation Programme Singapore (PIPS); one stream builds on CARES work on a previous PIPS project to create a methodology for digital twins for pharmaceutical process development, another stream will focus on using data-driven solutions to rapidly identify environmental impacts in the chemical supply chain.

CARES is also contributing to two projects in the Low-Carbon Energy Research (LCER) Phase 2 Programme, one hosted by NUS and one hosted by NTU.

CARES celebrated its first decade in Singapore in 2023 with a Scientific Showcase highlighting achievements in Digital Transformation, Chemical Technologies and Processes, From Emissions to Solutions, and Lifelong Learning. The scientific content from the event and highlights from 2023 can be viewed here: https://www.cares.cam.ac.uk/10anniversary/

This report is a summary of our last half-year of research progress. It includes scientific updates from each of our researchers, along with abstracts and figures from our recent publications.



OUTSTANDING WORK FROM THE LAST SIX MONTHS OF CAMBRIDGE CARES RESEARCH

Highlighted research outputs from October 2024 - March 2025

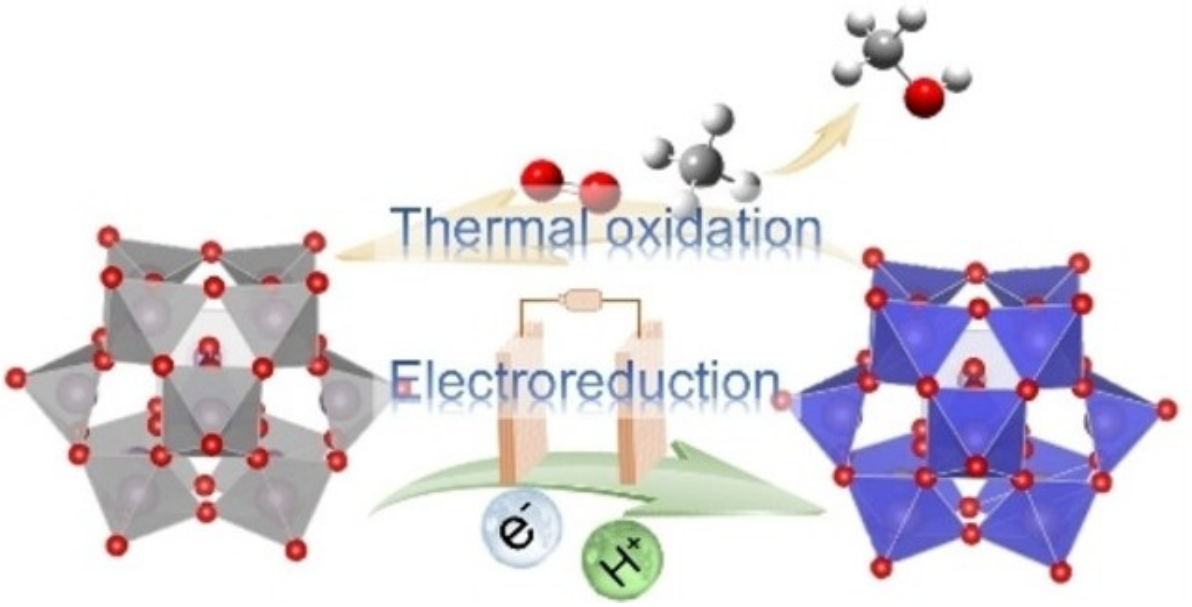
A selection of publications from across our programmes.

C4T: Electrothermal Conversion of Methane to Methanol at Room Temperature with Phosphotungstic Acid

Jinquan Chang, Sikai Wang, Max J. Hülsey, Sheng Zhang, Shi Nee Lou, Xinbin Ma, and Ning Yan,
Angewandte Chemie International Edition

DOI: 10.1002/anie.202417251

Abstract: Traditional methods for the aerobic oxidation of methane to methanol frequently require the use of noble metal catalysts or flammable H_2-O_2 mixtures. While electrochemical methods enhance safety and may avoid the use of noble metals, these processes suffer from low yields due to limited current density and/or low selectivity. Here, we design an electrothermal process to conduct aerobic oxidation of methane to methanol at room temperature using phosphotungstic acid (PTA) as a redox mediator. When electrochemically reduced, PTA activates methane with O2 to produce methanol selectively. The optimum productivity reaches 29.45 with approximately 20.3 % overall electron yield. Under continuous operation, we achieved 19.90 catalytic activity, over 74.3 % methanol selectivity, and 10 hours durability. This approach leverages reduced PTA to initiate thermal catalysis in solution phase, addressing slow methane oxidation kinetics and preventing overoxidations on electrode surfaces. The current density towards methanol production increased over 40 times compared with direct electrochemical processes. The in situ generated hydroxyl radical, from the reaction of reduced PTA and oxygen, plays an important role in the methane conversion. This study demonstrates reduced polyoxotungstate as a viable platform to integrate thermo- and electrochemical methane oxidation at ambient conditions. .



C4T: Support-Free Iridium Hydroxide for High-Efficiency Proton-Exchange Membrane Water Electrolysis

Yubo Chen, Chencheng Dai, Qian Wu, Haiyan Li, Shibo Xi, Justin Zhu Yeow Seow, Songzhu Luo, et al., *Nature Communications*

DOI: 10.1038/s41467-025-58019-7

Abstract: The large-scale implementation of proton-exchange membrane water electrolyzers relies on high-performance membrane-electrode assemblies that use minimal iridium (Ir). In this study, we present a support-free Ir catalyst developed through a metal-oxide-based molecular self-assembly strategy. The unique self-assembly of densely isolated single IrO_6H_8 octahedra leads to the formation of μm-sized hierarchically porous Ir hydroxide particles. The support-free Ir catalyst exhibits a high turnover frequency of 5.31 s^{-1} at 1.52 V in the membrane-electrode assembly. In the corresponding proton-exchange membrane water electrolyzer, notable performance with a cell voltage of less than 1.75 V at 4.0 A cm^{-2} (Ir loading of 0.375 mg cm^{-2}) is achieved. This metal-oxide-based molecular self-assembly strategy may provide a general approach for the development of advanced support-free catalysts for high-performance membrane-electrode assemblies.

C4T: Advances in CO_2 Reduction on Bulk and Two-Dimensional Electrocatalysts: From First Principles to Experimental Outcomes

Raghavendra Rajagopalan, Shivam Chaturvedi, Neeru Chaudhary, Abhijit Gogoi, Tej S. Choksi, and Ananth Govind Rajan, *Current Opinion in Electrochemistry*

DOI: 10.1016/j.coelec.2025.101668

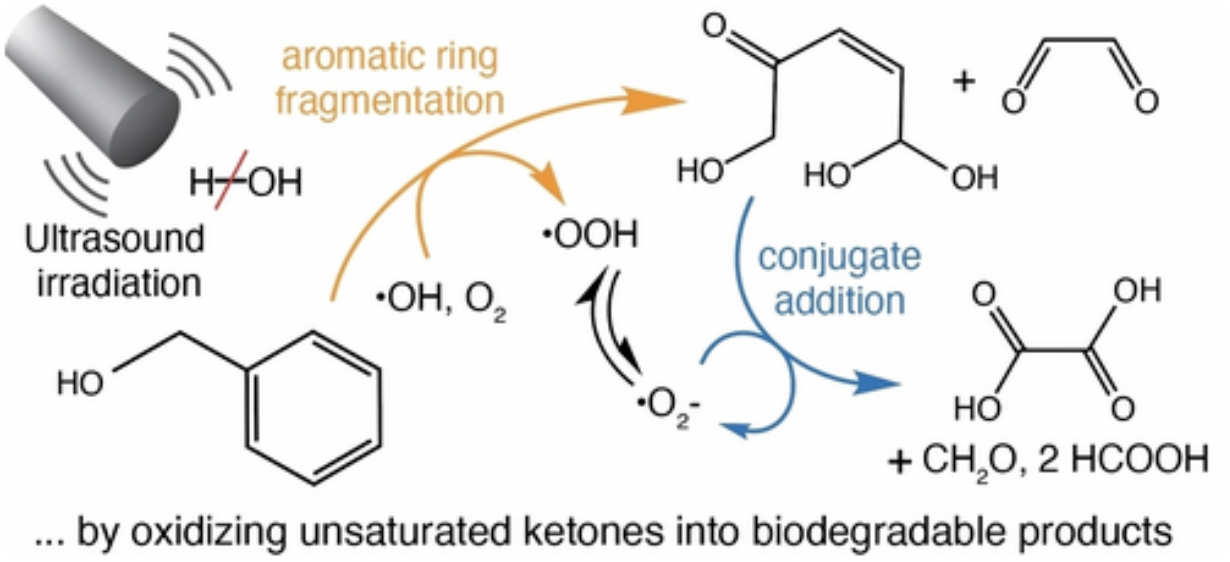
Abstract: Designing catalyst materials for the electrochemical carbon dioxide reduction reaction (CO_2RR) requires an understanding of the underlying thermodynamics and kinetics. In this review, we discuss the characteristics of two-dimensional (2D) and bulk materials, which distinguish their catalytic properties. We map catalyst performance in the faradaic efficiency–applied potential space for various hydrocarbons and oxygenates on these catalyst classes. We explain different approaches for modeling catalytic CO_2RR, such as the computational hydrogen electrode, grand canonical (GC) potential kinetics, and GC density functional theory, with the latter-most accurately capturing potential-dependent kinetics. We review recent attempts made to break scaling relationships between intermediate adsorption energies and describe unique features found in 2D materials. Finally, we compare kinetics on both material classes using microkinetic modeling. We conclude that future studies should focus on realistic simulations of the electrode–electrolyte interface and combining the favorable properties of 2D and bulk materials to engineer high-performance CO_2RR catalysts.

C4T: The Roles of Hydroxyl Radicals and Superoxide in Oxidizing Aqueous Benzyl Alcohol Under Ultrasound Irradiation

Ari F. Fischer, Teseer Bahry, Zhangyue Xie, Roberto Batista da Silva Junior, Kaicheng Qian, Renhong Li, James Kwan, et al., *ChemSusChem*

DOI: 10.1002/cssc.202500097

Abstract: The abatement of aromatic pollutants in water requires their oxidation to nontoxic products by resource-intensive reactions with hydroxyl radicals (·OH). We elucidate the mechanisms of ·OH-induced aromatic ring degradation by combining kinetic measurements, electron paramagnetic resonance spectroscopy, density functional theory calculations, and kinetic modelling. We demonstrate that benzyl alcohol (a model aromatic compound) is oxidized by ·OH radicals, generated by ultrasonic irradiation in an O_2-rich environment, into aromatic compounds (benzaldehyde and phenol derivatives) and C1–C2 oxygenates (formic acid, glyoxal, and oxalic acid). Through pathways akin to atmospheric chemistry, these ·OH radicals de-aromatize and fragment benzyl alcohol, producing 5-hydroxy-4-oxo-pentenal and other dicarbonyl products. Unique to the aqueous phase, however, superoxide ($\cdot O_2^-$) forms by ·OOH deprotonation, which is generated by ultrasound (alongside ·OH) and as a byproduct of ·OH-benzyl alcohol reactions. $\cdot O_2^-$ acts as a nucleophile, oxidizing 5-hydroxy-4-oxo-pentenal into oxalic acid and C1 oxygenates via aldehyde and ketone intermediates. This process regenerates $\cdot O_2^-$ and does not consume ·OH, thereby further degrading ring fragmentation products while preserving ·OH to activate the refractory aromatic ring of benzyl alcohol. These nucleophilic $\cdot O_2^-$ reactions can therefore reduce the energy and number of chemical initiators needed to degrade aromatic compounds, thus advancing ·OH-based oxidation processes in water treatment.

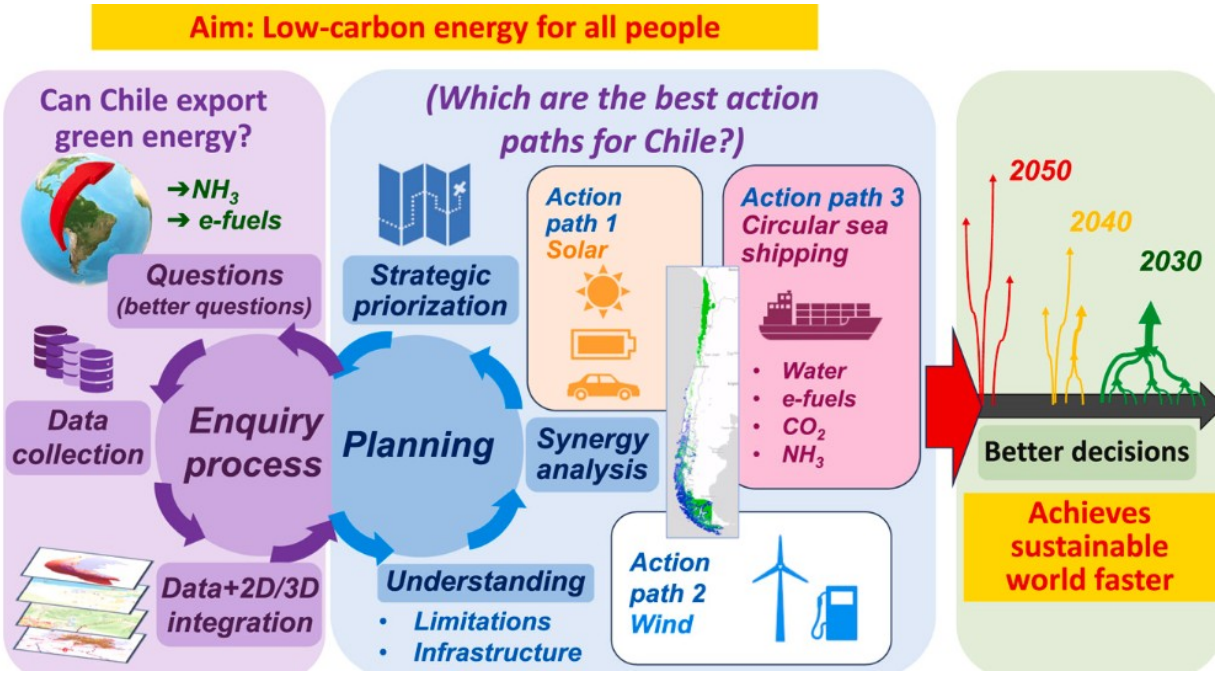


C4T: An Analysis of Renewable Energy Resources and Options for the Energy Transition in Chile

Andrea M. Oyarzún-Aravena, Jiying Chen, George Brownbridge, Jethro Akroyd, and Markus Kraft,
Applied Energy

DOI: 10.1016/j.apenergy.2024.125107

Abstract: This study analyses renewable energy resources, infrastructure, and practical options to accelerate the energy transition and unlock Chile's potential as an exporter of renewable energy and products. We analyse data on the potential of wind and solar energy to determine the best areas for renewable projects. The progress of the energy transition occurring in Chile is reviewed in the context of historical events. The abundant renewable energy resources far exceed current demand and offer exceptional harvesting conditions. However, geographical limitations and a lack of enabling infrastructure may limit the participation of Chile in the world net-zero economy. A comparison is made with the UK to provide a broader perspective. This identifies order-of-magnitude differences in the power available in different locations, highlighting the importance of considering where best to deploy limited resources. International cooperation is required to make the best use of the available renewable energy. Three practical international options to unlock Chile's potential are discussed. Further technical-economic assessment of these energy-transition acceleration paths is recommended. The data and results are integrated into a set of 2D/3D visualisations, facilitating visual insights and enabling a comprehensive understanding of the challenges and opportunities facing Chile.

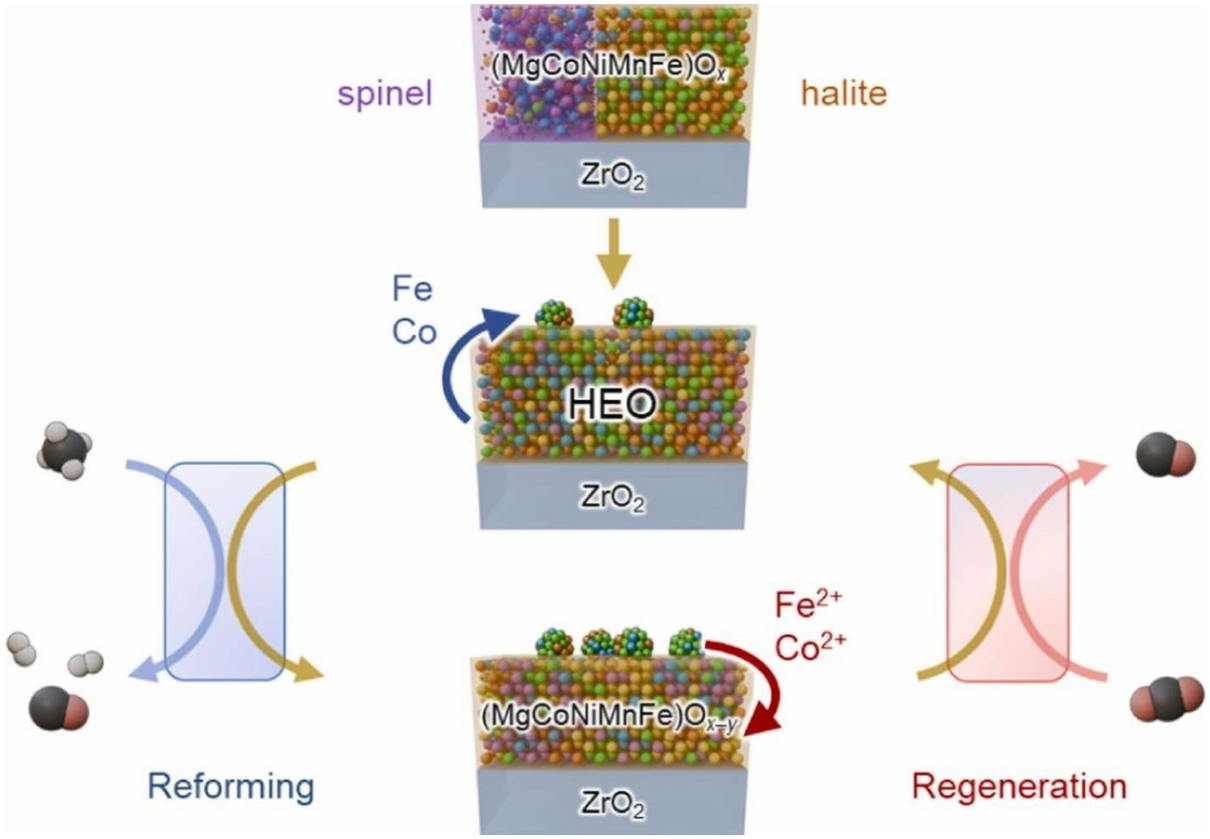


C4T: Halite-Structured (MgCoNiMnFe)O High Entropy Oxide (HEO) for Chemical Looping Dry Reforming of Methane

Shao Yu, Chao Wu, Shibo Xi, Preston Tan, Xianyue Wu, Syed Saqline, and Wen Liu, *Applied Catalysis B: Environment and Energy*

DOI: 10.1016/j.apcatb.2024.124191

Abstract: The configurational disorder of high entropy oxides (HEOs) promotes the reversible exsolution–redissolution of constituent metal species. This unique feature could be exploited to facilitate cyclic lattice oxygen storage and exchange. Herein, we report an in situ generated, halite-structured (MgCoNiMnFe)Ox HEO, which simultaneously functions as a redox catalyst and an oxygen carrier for dry reforming of methane in a chemical looping process (CL–DRM). Accordingly, the (MgCoNiMnFe)Ox/ZrO_2 HEO catalyst exhibits outstanding DRM activity, syngas selectivity and cyclic stability compared to medium-entropy oxides and bimetallic oxides over 100 CL–DRM cycles at 800°C. XRD analysis verified the entropy-mediated preservation of the alloy/HEO/ZrO_2 catalytic structure over CL–DRM cycles. XAFS studies revealed the reversible and cyclic evolution–dissolution of Ni, Fe, Co over redox cycles. The exsolved NiFeCo nanoalloy exhibited high efficiency in activating CH_4. This study has demonstrated the potential applications of HEO-based catalysts in efficient chemical looping processes.

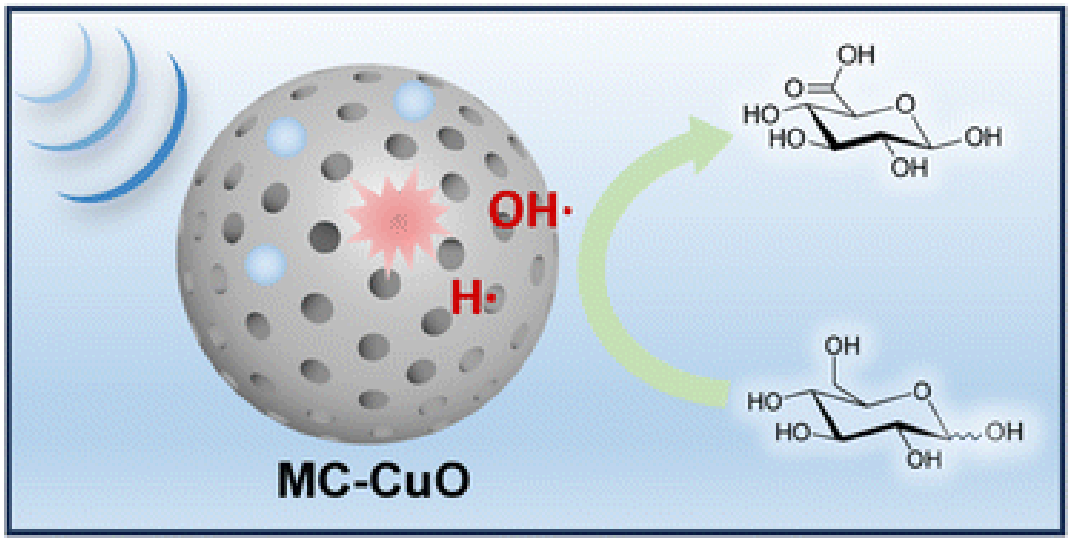


C4T: Boosting Energy Efficiency and Selectivity of Glucose Oxidation toward Glucuronic Acid in High-Frequency Ultrasound Using Multicavity CuO Catalytic Cavitation Agents

Zhangyue Xie, Valarmathi Mahendran, Umesh S. Jonnalagadda, Qianwenhao Fan, Xiaoqian Su, Ari F. Fischer, Mingwu Tan, et al., *Green Chemistry*

DOI: 10.1039/D4GC03775H

Abstract: Sonochemistry has shown potential to facilitate chemical conversion under near-ambient conditions in water without any chemical additive or other external stimulus. With the help of catalytic cavitation agents, the generation of radicals from ultrasound-induced inertial cavitation can be enhanced and utilized more efficiently for selective chemical transformations. In this study, multicavity CuO (MC-CuO) microparticles were prepared and employed as catalytic cavitation agents to promote spatially selective cavitation and simultaneously catalyze sonochemical oxidation of glucose. Accordingly, the rate of production of OH radicals by sonolysis of water, inferred from titration, was directly related to the cavitation energy, which was determined by analyzing the acoustic signal during pulsed irradiation of 500 kHz ultrasound. Two reaction pathways for glucose oxidation were identified. First, the generation of OH radicals and possibly other reactive oxygen species in the bulk aqueous phase resulted in the formation of gluconic acid, together with other byproducts of C–C bond cleavage and ring opening. Second, the generation of OH radicals in close proximity to CuO resulted in the formation of glucuronic acid with the six membered ring preserved. The present study demonstrates that by appropriately controlling the acoustic parameters (e.g. duty cycle, peak negative pressure and irradiation time) and reaction conditions (e.g. gas atmosphere and the addition of catalytic cavitation agent), it is possible to steer the selectivity of sono-oxidation of glucose towards glucuronic acid, the most value-added product, whilst minimizing the energy input to drive the sonochemical oxidation reaction.

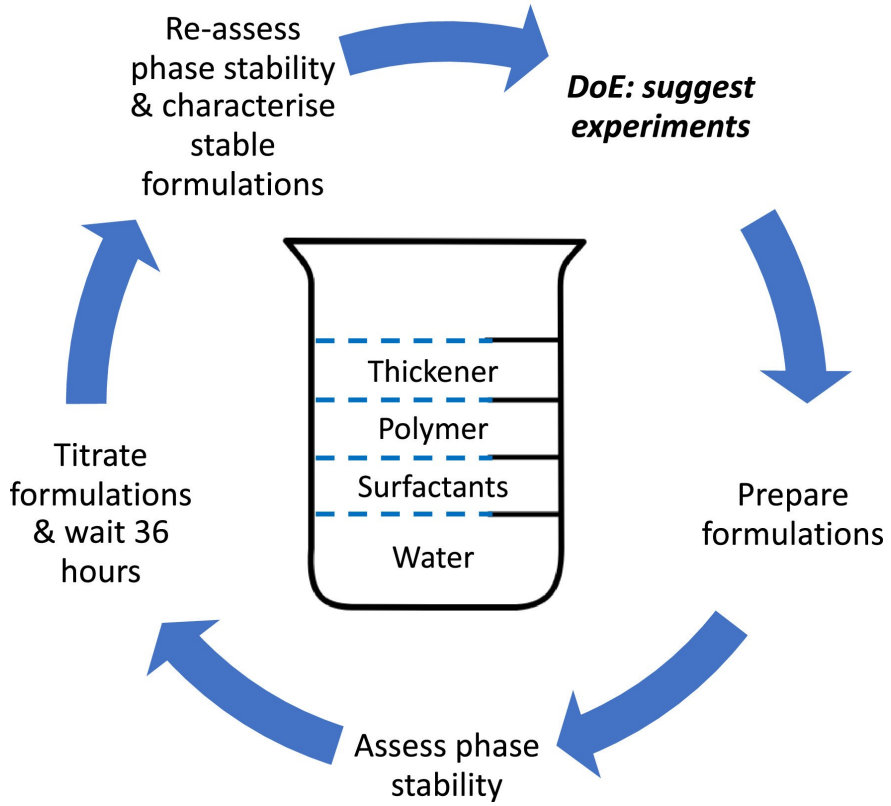


C4T: Machine Learning-Guided Space-Filling Designs for High Throughput Liquid Formulation Development

Aniket Chitre, Daria Semochkina, David C. Woods, and Alexei A. Lapkin, *Computers & Chemical Engineering*

DOI: 10.1016/j.compchemeng.2025.109007

Abstract: Liquid formulation design involves using a relatively limited experimental budget to search a high-dimensional space, owing to the combinatorial selection of ingredients and their concentrations from a larger subset of available ingredients. This work investigates alternative shampoo formulations. A space-filling design is desired for screening relatively unexplored formulation chemistries. One of the few computationally efficient solutions for this mixed nominal -continuous design of experiments problem is the adoption of maximum projection designs with quantitative and qualitative factors (MaxProQQ). However, such purely space-filling designs can select experiments in infeasible regions of the design space. Here, stable products are considered feasible. We develop and apply weighted-space filling designs, where predictive phase stability classifiers are trained for difficult-to-formulate (predominantly unstable) sub-systems, to guide these experiments to regions of feasibility, whilst simultaneously optimising for chemical diversity by building on MaxProQQ. This approach is extendable to other mixed-variable design problems, particularly those with sequential design objectives.



HD_4: Harnessing Street Shade to Mitigate Heat Stress: An in-Situ Parallel Investigation under Extreme Heat Conditions in Tropical Singapore

Lei Xu, Ronita Bardhan, Hao Mei, Srilalitha Gopalakrishnan, Xing Zheng, and Thomas Schroepfer,
Science of The Total Environment

DOI: 10.1016/j.scitotenv.2024.177864

Abstract: In the face of global rising temperatures and excessive urban heat, developing effective heat mitigation strategies has become increasingly urgent. Street shade, a typical cooling shelter for urban dwellers, has been primarily investigated for outdoor thermal comfort but not extensively under extreme heat conditions. This study explores the cooling efficacy of diverse street shade types in mitigating urban heat, thereby facilitating cities and their residents' adaptation to climatic shifts. We conducted in-situ measurements during an extremely hot afternoon, measuring thermal and visual environments across 20 pairs of parallel sites (sunlit vs. shaded) in a high-density district of tropical Singapore. Subsequently, we analyzed thermal comfort, represented by the Universal Thermal Comfort Index (UTCI), heat stress risks, and view factors of the sky, greenery, and buildings, and their interaction with heat stress relief. Our findings highlight three key points: Firstly, all street shade types improved outdoor thermal conditions, with average decreases of 0.8 °C in air temperature, 10.0 °C in mean radiant temperature, and 3.1 °C in UTCI. Secondly, street shade generally reduced heat stress severity by 20 % in the 'very strong heat stress' category and 12 % in the 'strong heat stress' category. Thirdly, the cooling efficacy of street shade was not solely dependent on changes in any single view factor. The results demonstrate the significant cooling benefits provided by street shade during extreme heat conditions. This study not only underscores the crucial role of street shade in mitigating heat stress but also offers valuable guidance to urban planners and designers in creating more liveable, sustainable, and climate-adaptive cities.

C4T

CAMBRIDGE CENTRE FOR CARBON REDUCTION IN CHEMICAL TECHNOLOGIES (C4T)

C4T is the flagship programme at CARES investigating carbon reduction solutions in the areas of sustainable reaction engineering, electrochemistry, sustainable energy, maritime decarbonisation, carbon policy, and digital networks. The current impact-focused projects have been marked as "CN" and will be guided by local agency stakeholders using research developed from the first two phases of C4T.

C4T leads:

Professor Markus KRAFT
University of Cambridge

Professor Rong XU
Nanyang Technological University

Professor Ning YAN
National University of Singapore

SUSTAINABLE REACTION ENGINEERING

CN2: Integrated carbon capture and conversion – from fundamental understanding to hypothesis-driven synthesis of high performance dual functional materials

Assoc Prof Wen LIU (Paul) (NTU)

Asst Prof Tej CHOKSI (NTU)

Ms Xianyue WU (Research Assistant, CARES) has been actively working on the development of CO_2 capture and in-situ hydrogenation process using Ni/alkaline earth metal carbonate dual-function materials (DFMs). She has been investigating mechanistic and kinetics studies on the hydrogenation of the Ni-amorphous $CaCO_3$-based dual-function materials (DFMs). She studied the effects of H_2 partial pressure on the hydrogenation of Ni/$CaCO_3$ DFM (Figure 1.1), and the decomposition of carbonate species during the process (Figure 1.2). Moreover, she is helping

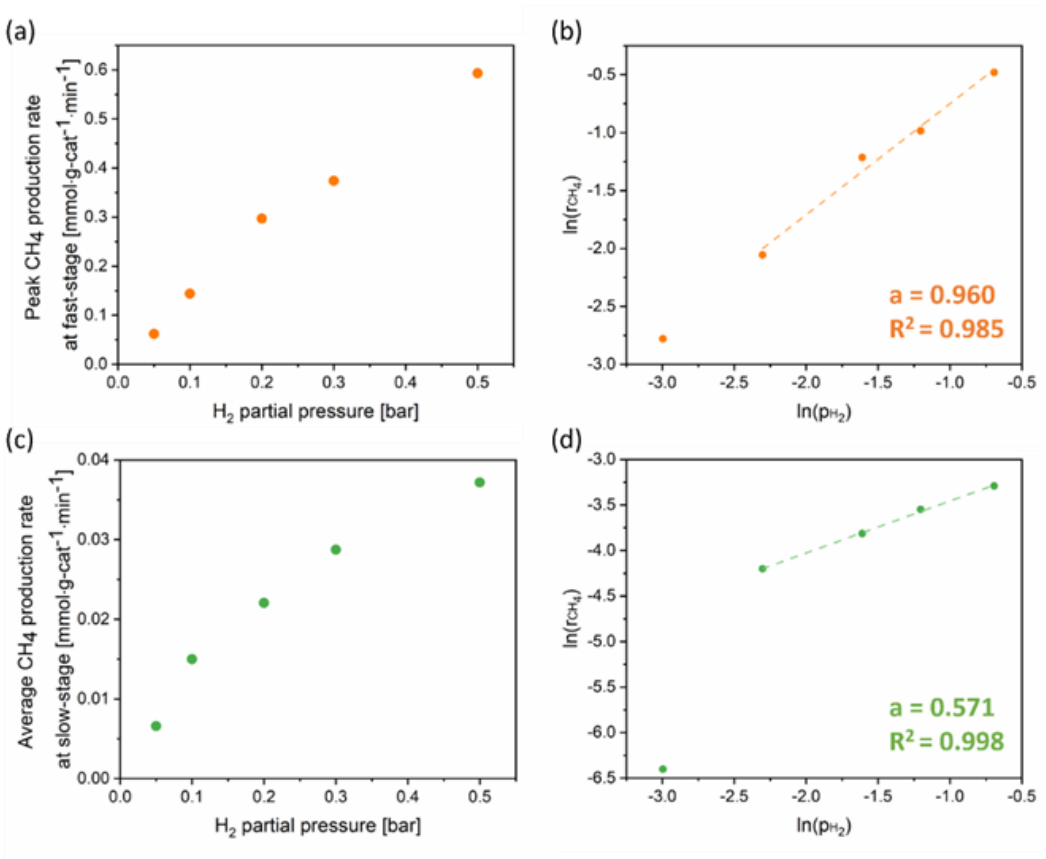


Figure 1.1: a) Peak CH_4 production rate during fast-stage hydrogenation on 2Ni/ACC in different H_2 partial pressures and (b) the corresponding Arrhenius plot; (c) Average CH_4 production rate during slow-stage hydrogenation on 2Ni/ACC in different H_2 partial pressures and (d) the corresponding Arrhenius plot.

Ms Xianyue WU

with some scale-up tests on CO_2 processing agents (CDPA). She analysed the CO_2 adsorption capacity of CDPA in a humid atmosphere with a light source (Figure 1.3).

Ms Wu is also working with Alganaza Pte. Ltd. to do carbon dioxide processing agent (CDPA) tests. She helped with packed bed experiments (Figure 1.3), long-term batch CO_2 adsorption tests (Figure 1.4), and isotope C^{13} labelling (Figure 1.5) conducted in CARES. She was also responsible for the summary report writing with her supervisor, **Assoc Prof Wen LIU (Paul) (PI, NTU)**.

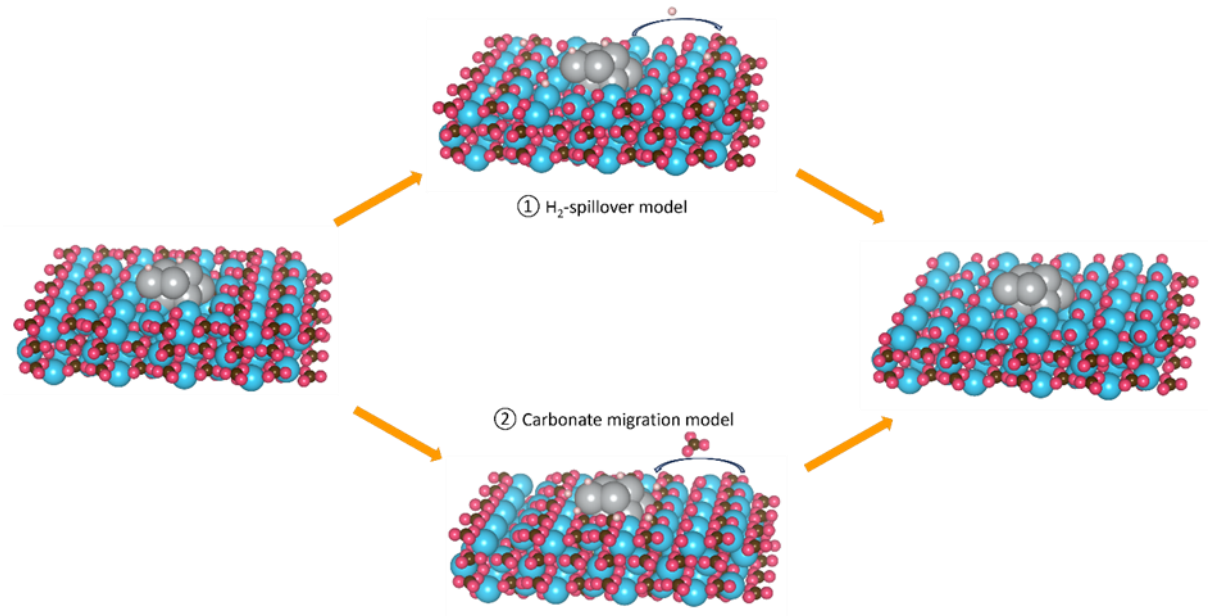


Figure 1.2: Hypothesised reaction model of slow-stage hydrogenation of Ni/$CaCO_3$ DFMs

Ms Xianyue WU

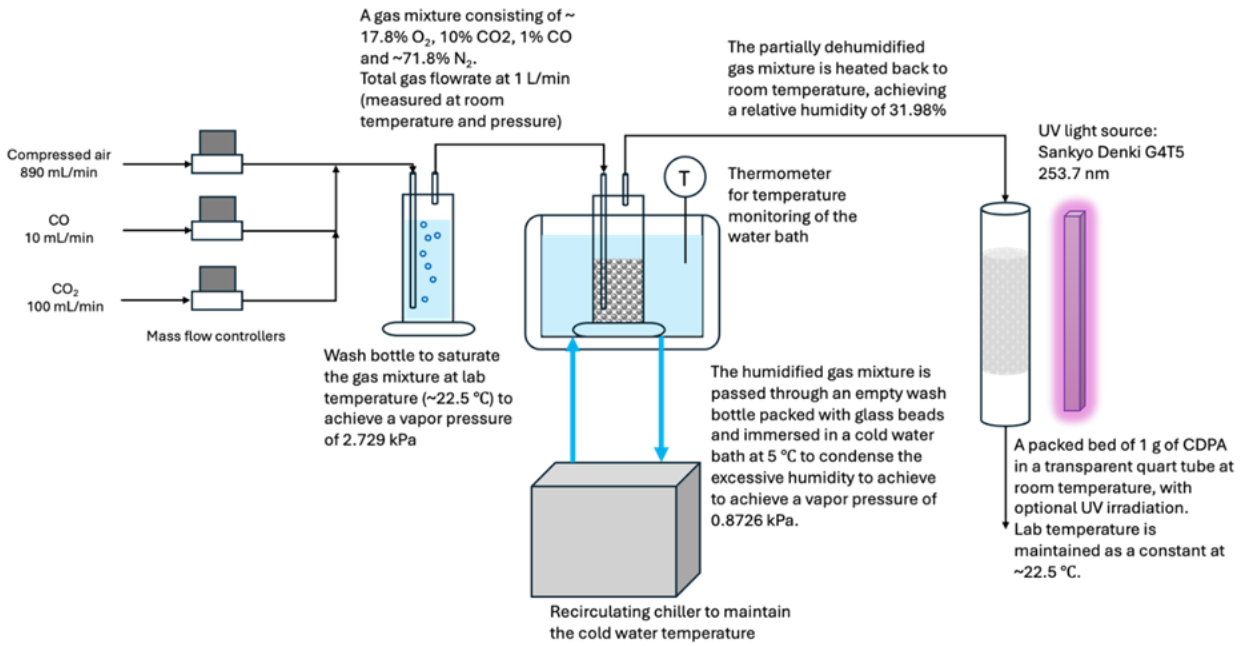


Figure 1.3: Schematic illustration of the packed bed setup with gas inlet with controlled humidity and UV light irradiation.

Ms Xianyue WU

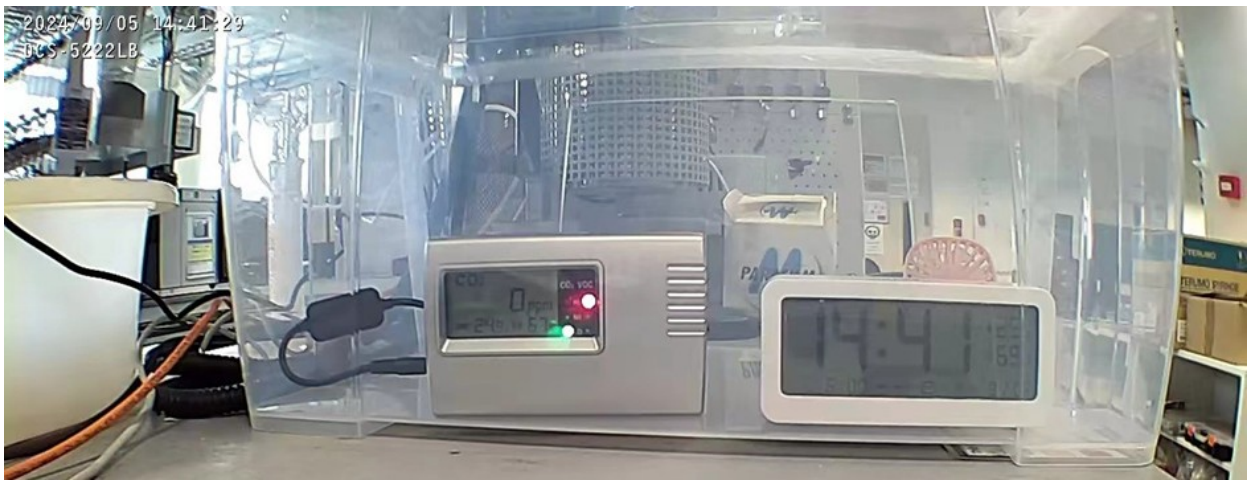


Figure 1.4: Photo of the setup for CO_2 removal experiments in an enclosure.

Ms Xianyue WU

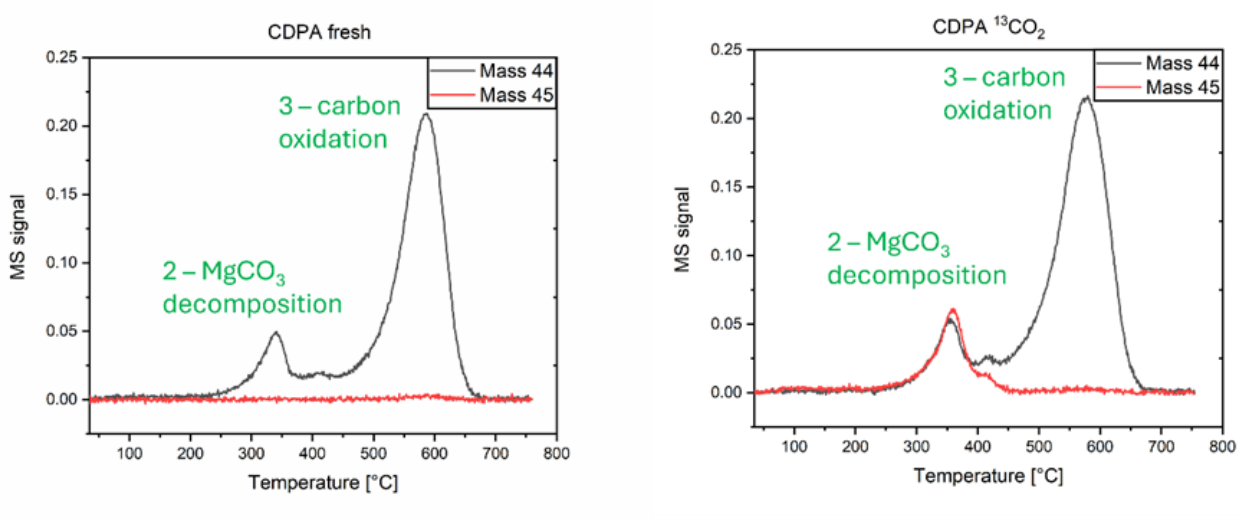


Figure 1.5: MS signal of MS = 44 and 45 during the TPO of fresh and $^{13}CO_2$ treated CDPA sample

Ms Xianyue WU

ELECTROCHEMISTRY

CN15: Advanced low carbon manufacturing technologies for localised disinfectant production, using novel electrode-membrane architectures

Prof Adrian FISHER (CAM)

Prof Zhichuan XU (Jason) (NTU)

Assoc Prof Sui ZHANG (NUS)

Assoc Prof Sui ZHANG's (PI, NUS) group has continued to work on the challenging task of separating molecules with similar sizes but different shapes. Here, conjugated microporous polymer (CMP) membranes with narrowly distributed network pores are prepared by diffusion-modulated electropolymerisation. This approach precisely controls the monomer diffusion and coupling processes, regulating the crosslinking degree to prevent broad aggregate pores and microporous defects. By altering carbazole-based backbones, pore size and pore connectivity are adjusted. The rigid and interconnected confinements restrict molecular rotation and vibration, enforcing consistent shapes and orientations. This enables the separation of solute molecules (≈1000 g mol^{-1}) with linear and bulky shapes, achieving separation factors of up to 134. When pore size is reduced to angstrom scale (≈5 Å), molecular shape significantly influences organic liquid transport. The CMP membranes demonstrate all-liquid phase separation of linear/branched alkane isomers (<100 g mol^{-1}), enriching hexane to 63.35 mole% from equimolar isomer mixture and achieving permeance orders of magnitude higher than those of state-of-the-art membranes.

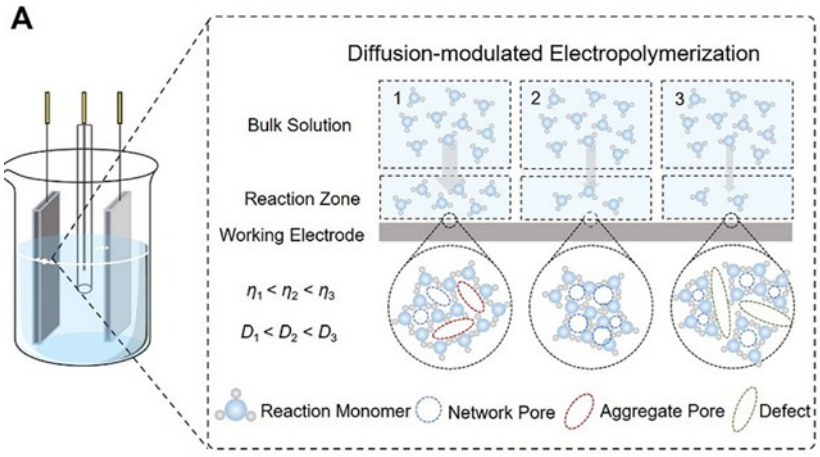


Figure 2.1: A figure illustrating the diffusion-modulated electropolymerisation of CMP membranes.

Assoc Prof Sui ZHANG

CN26: New electrosynthesis routes for production of organic acids, e.g., oxalic, lactic, benzoic

Prof Adrian FISHER (CAM)

Prof Zhichuan XU (Jason) (NTU)

Dr Chencheng DAI's (Research Fellow, NTU) research has been focusing on two parts.

The first is hydrogen production from methanol electrolysis, demonstrating the highly efficient utilisation of electricity energy to convert methanol to hydrogen at low temperature and ambient pressure. A stable, industrial-level current density of 200 mA cm^{-2} was achieved in a PEME with a low cell potential of only 0.44 V, corresponding to an energy efficiency of 81.9%. Additionally, the produced hydrogen is separated from other products as the HER and MOR occur in different chambers and exit through different outlets. This design simplifies the product separation and purification processes.

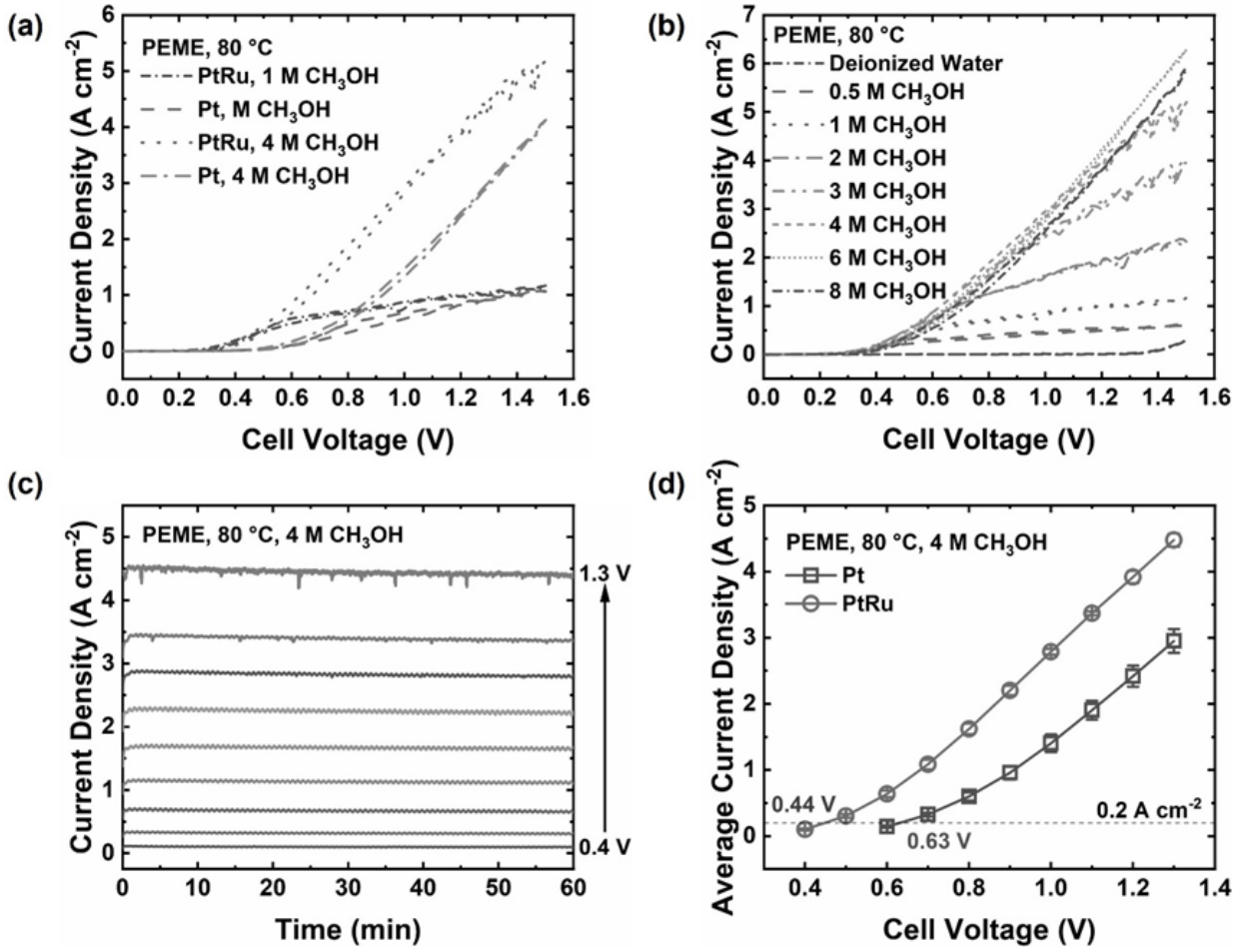


Figure 2.2: (a) Comparison of cyclic voltametric curves in methanol solutions of PEM electrolyser with 3 mg_{Pt} cm^{-2} 40 wt% Pt/C and 60 wt% PtRu/C anode catalysts at 80 °C. (b) Cyclic voltametric curves (10 mV s^{-1}) in methanol solution of various concentrations, and (c) chronoamperometric curves at various cell voltages with 4 M methanol of the PEM electrolyser solution with 3 mg_{Pt} cm^{-2} 60 wt% PtRu/C at 80 °C. (d) Comparison of the polarisation curves in 4 M methanol solution of PEM electrolyser with 3 mg_{Pt} cm^{-2} 60 wt% PtRu/C anode catalysts at 80 °C.

Dr Chencheng DAI

Dr Dai's second research focus is on electrochemical ammonia cracking. Various noble catalysts have been screened for electrochemical ammonia oxidation reaction. Theoretical studies suggest the presence of competitive energetics between NH_x dehydrogenation and N-N coupling in AOR, revealing a volcano relationship between the energy barrier of dehydrogenation steps and the potential limiting step. The surface oxidation of catalysts near the apex of volcano, including Pt, Ir, and Pd, results in unfavourable NH_x dehydrogenation steps, suggesting oxidative deactivation mechanism. Amongst all catalysts studied, Pt is selected as it uniquely synergises moderate dehydrogenation energetics, a high regeneration capability via electrode polarity reversal, and excellent corrosion resistance in ammonia electrolytes. A techno-economic analysis was conducted, and the hydrogen production cost is 1.29 USD per kg, which is significantly lower than the reported hydrogen production cost via traditional thermal cracking methods (~ 5 USD per kg).

Dr Qikai SHEN's (Research Fellow, NTU) main research interest lies in the development of electrocatalysts for ammonia-based energy systems. Over the past six months, he has focused on designing and evaluating a new catalyst for direct ammonia fuel cells (DAFCs), with the aim of overcoming the sluggish kinetics of the ammonia oxidation reaction (AOR). His work explores strategies to simultaneously enhance ammonia activation and hydroxide adsorption, both of which are critical to improving reaction efficiency. He has carried out a combination of experimental studies and theoretical analyses to investigate the catalyst's performance and underlying mechanisms. These efforts have resulted in notable improvements in electrocatalytic activity under low-temperature fuel cell conditions. Dr Shen is currently working on further optimising the catalyst-support interface and integrating the material into membrane electrode assemblies, to advance its application in practical DAFC systems. This work contributes to developing efficient, carbon-neutral energy technologies based on ammonia as a sustainable fuel.

MARITIME DECABONISATION

CN1: Air pollutant measurements with aerial devices

Prof Markus KRAFT (CAM)
Prof Epaminondas MASTORAKOS (CAM)
Assoc Prof Liya YU (NUS)

The project aims to explore the suitability of new sensors (such as those for nitrogen oxides, ammonia, methanol, and others) for use in drones or Unmanned Aerial Vehicles (UAVs) within ports by building on the success of measuring particulate matter levels with a drone, and on characterising and apportioning particulate matter using available sensor data.

During this reporting period, air quality measurements were proposed at several locations across Singapore, selected to represent distinct residential and industrial environments, as illustrated in Figure 3.1. Following this, data collection was successfully conducted at two of the locations: one in proximity to maritime and industrial activities near Jurong Island (Teban Vista),

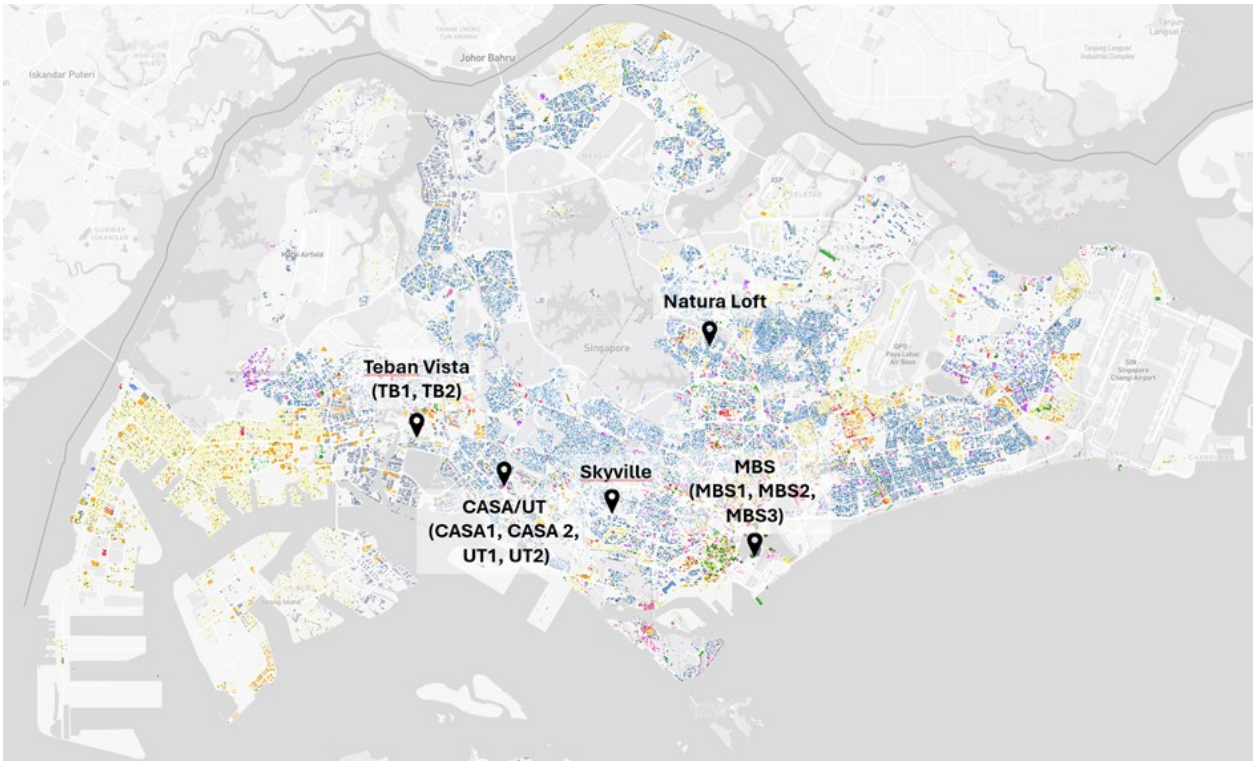


Figure 3.1: Proposed measurement locations include sites influenced by maritime activity (Marina Bay Sands), combined maritime and industrial activity (Teban Vista), and residential environments (CASA, University Town, Skyville, and Natura Loft). The locations are visualised using The World Avatar (TWA) framework, which provides an interactive and semantically enriched base map for integrating and analysing spatial and environmental data.

Dr Mutian MA

and another at a nearby residential location (CASA/University Town). Data collection at the other locations is in progress.

The MicroAeth Model MA200 instrument was employed to measure concentrations of black carbon (BC) and brown carbon (BrC). BC is a particulate pollutant emitted from various combustion sources, including industrial processes and vehicular traffic. BrC, a subset of carbonaceous particles, is typically associated with biomass combustion and shipping emissions, and is also considered a significant contributor to climate forcing.

Figure 3.2 displays the average concentrations of equivalent black carbon (eBC), defined as BC measured using light absorption techniques. These concentrations were recorded at varying altitudes and are supplemented with data from aerial sampling campaigns, which was documented in the previous report.

The observed eBC concentration ranges were consistent across multiple sampling days and were comparable to values reported in the literature and those reported by the National Environment Agency (NEA) monitoring stations. Vertical concentration profiles varied across sampling days at the same location (designated as "site + number," e.g., CASA1 and CASA2).

Notably, elevated eBC concentrations recorded at higher altitudes (e.g., 20th to 40th storeys), suggests that residents living at such elevations may be subject to increased exposure.

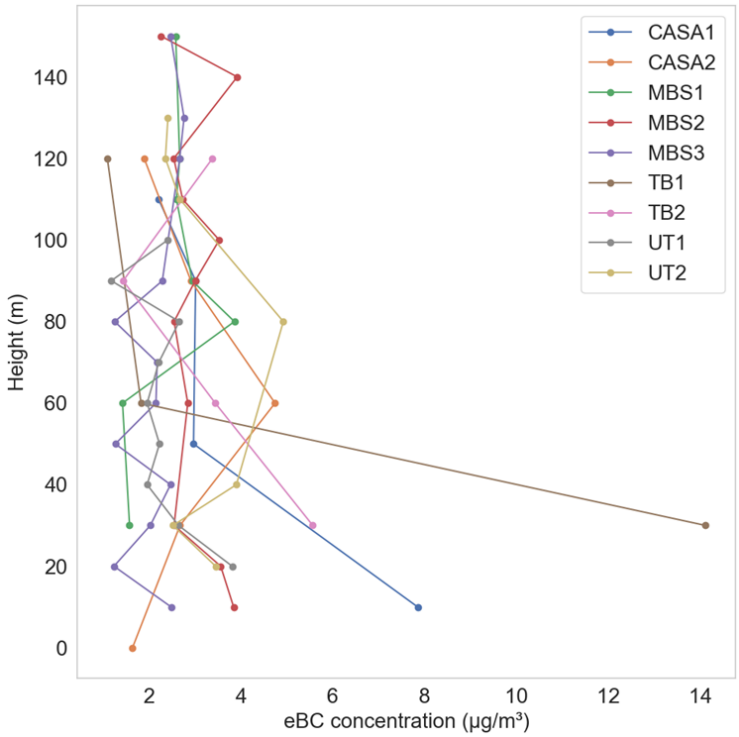


Figure 3.2: Box plot depicting vertical profiles of eBC concentrations at various sites. Data are categorised by height and measurement date (e.g., CASA1 and CASA2 represent measurements taken on two separate days at the CASA site).

Dr Mutian MA

CN14: Alternative marine fuel engine modelling

Prof Epaminondas MASTORAKOS (CAM)

Dr Li Chin LAW (Research Fellow, CARES) has been involved in the research project with Laskaridis Shipping and METIS Cybertechnology to better analyse shipping performance. The two years of historical data (2023 and 2024) provided by Laskaridis Ship Management company was analysed using newly developed in-house data analytics tools. The performance of reference bulk carrier was evaluated by analysing the vessel's operational profile and voyage patterns. Using

the historical data, an optimal conceptual design was developed to retrofit the vessel with alternative fuel systems and onboard carbon capture (OCCS) technologies. The design avoided system overdesign and lowered Laskaridis' investment costs. Transitioning to alternative fuels is feasible if available space is used efficiently and the added deadweight is evenly distributed to minimise impacts on ship stability. Additional safety features must also be integrated to manage associated hazards.

Furthermore, selected solutions should demonstrate low lifecycle emissions to comply with evolving regulatory requirements. Economic viability depends on several factors, including current market prices of alternative fuels, capital expenditure (CAPEX) for fuel containment systems, and the cost of capture technologies. Additionally, emissions regulations play a significant role in accelerating the adoption of low-carbon alternatives. Low-emission transitions increase both operational (OPEX) and capital costs, policy instruments such as Fuel EU Maritime and the IMO's GHG Fuel Intensity (GFI) standards create strong financial incentives. These penalty- and reward-based systems not only impose substantial carbon costs but also offer potential revenue streams, further enhancing the economic attractiveness of investing in low-carbon technologies.

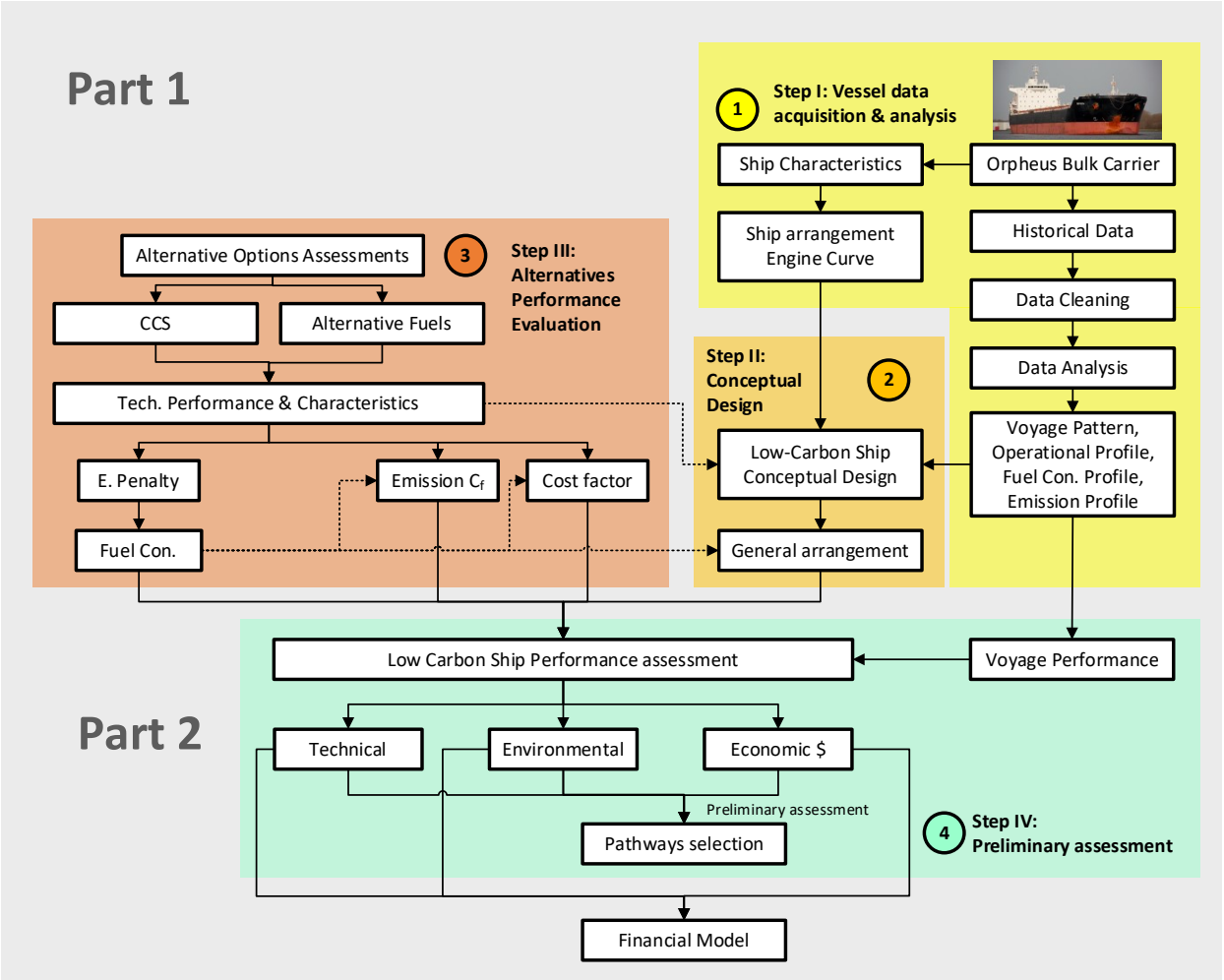


Figure 3.3: The research is divided into two parts. The first part of the study (Step 1 to Step 3) analysed ship data to understand the performance of the reference vessel, followed by conceptual design to retrofit the vessel ship for alternative fuels and CCS; lastly, the technical, environmental and economic aspects were discussed. In the second part, suitable low-carbon alternatives were selected, and the financial model was projected across 25 operational years.

Dr Li Chin LAW

CARBON POLICY

CN17: Extend internal carbon tax work to develop carbon pricing policy insights for Singapore

Prof S VISWANATHAN (NTU)

Prof. S. VISWANATHAN (PI, NTU), **Dr J. Lemuel MARTIN (Research Fellow, NTU)**, and **Dr Yan WANG (Research Fellow, NTU)** continue their work on studying the impact of carbon taxes on carbon intensive industries in Singapore. They have completed a preliminary study for the maritime sector that focuses on the maritime fuel transition as a potential baseline for estimating carbon tax bounds and the subsequent downstream impact on goods. Initial findings suggest that onboard carbon capture systems are the cheapest clean technology option, inducing carbon tax bounds of around 124-146 USD/tCO_2. However, the corresponding price fluctuation induced by the imposition of taxes at this level do not deviate significantly from regular price volatility, implying that these costs can be directly passed down to customers without adopting decarbonisation measures. Dr Wang has also conducted an analysis on the effect of different carbon tax levels on electricity costs, with some preliminary analysis on the downstream impact on sectors such as the semi-conductor industry. An expansion of the study into the oil and gas industry is being planned as well.

Dr Martin continues to work with Prof Viswanathan on the paper "Evaluating Alternative Business Models for Solar Panel Adoption: A Game Theoretic Approach." Their findings show that under limited heterogeneity, customer choices do not distinguish between third-party ownership models for solar panels, only doing so when they are sufficiently heterogeneous from each other with respect to energy demand and/or generation. The manuscript is now being prepared for submission to academic journals. Dr Wang continues to work with Prof Viswanathan on the paper "Sustainability Reporting Quality and Carbon Emissions Reduction: the Role of Chief Sustainability Officer." Their findings suggest that the presence of a Chief Sustainability Officer (CSO) contributes positively to the quality of sustainability reporting, but does not significantly enhance actual sustainability performance, especially on the experimental side. Dr Wang has completed the manuscript, and the group are now preparing it for submission to academic journals.

CN23: Introducing next generation laboratory

Prof Markus KRAFT (CAM)

The project aims to develop a proof of concept to establish a global network of self-driving laboratories working together in real time to optimise the same process. This has the potential to accelerate progress towards achieving the Pareto front for a multi-objective optimisation problem, thereby reducing the time required to develop new chemicals in the research environment.

During this reporting period, substantial progress was achieved in the integration of experimental setup within The World Avatar (TWA). A digital twin of the experimental setup in the CARES Laboratory was successfully linked to a conceptual representation of the selected experiment using ontologies. This integration facilitated the retrieval of equipment status and experimental reaction data through SPARQL queries executed on the knowledge graph.

A similar configuration was implemented for the experimental setup in Cambridge, where the knowledge graph was adapted to reflect the specific hardware specifications of that site. Once connectivity was established, the selected experiment was executed concurrently in both laboratories. Experimental data points were generated and exchanged between the two sites in real time.

The collaborative experiment resulted in the generation of a Pareto front for cost-yield optimisation, with all experimental results systematically recorded and stored in the knowledge graph in accordance with the FAIR principles (Findable, Accessible, Interoperable, and Reusable). Data provenance is fully traceable and can also be retrieved using SPARQL queries.

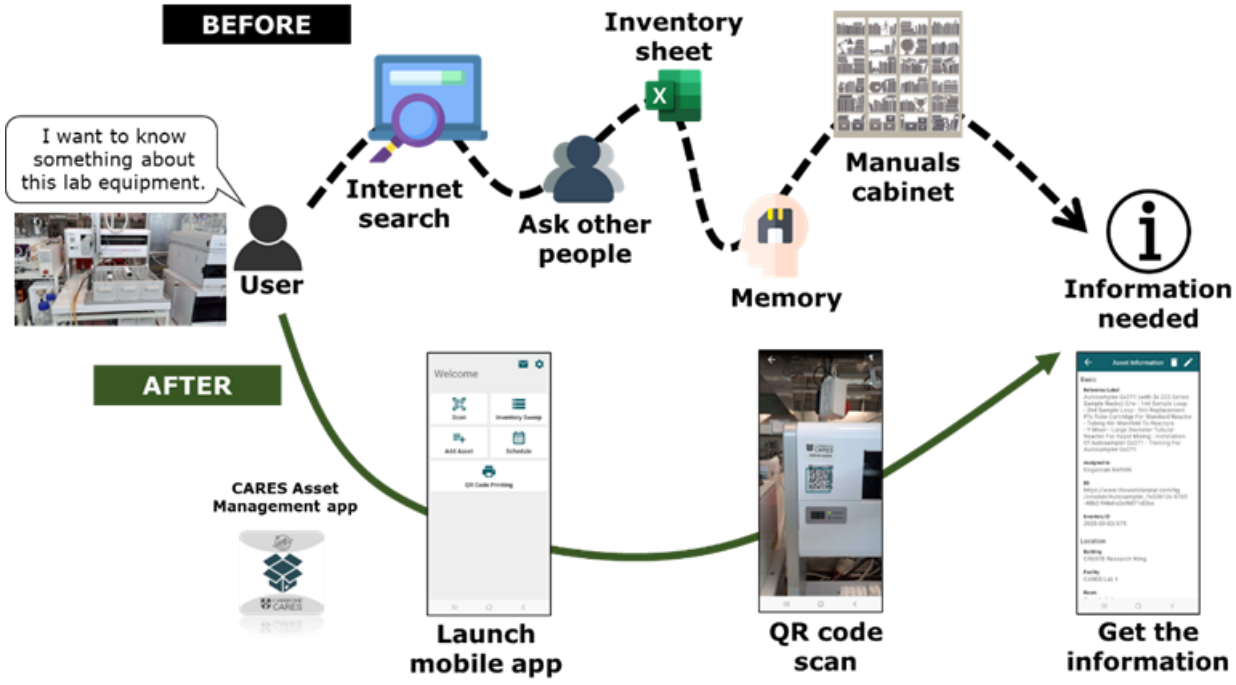


Figure 4.1: Improved workflow using the CARES Asset Management Mobile Application, which allows users to access equipment information via QR codes, replacing manual data retrieval methods.

To further enhance interoperability, the Open Platform Communications Unified Architecture (OPC-UA) standard was explored and incorporated into the Digital Laboratory Framework. This included the development of functionalities for reading from and writing to the knowledge graph using the OPC-UA protocol, thereby improving the flexibility and integration of laboratory components.

In parallel, the user interface was refined to support intuitive control and monitoring of the experimental environment. Specific enhancements were made to the mobile applications—particularly the Asset Management Mobile Application—to facilitate more effective interaction with the automated experimental setup.

CN24: Developing the Automated Lab of the Future

Prof Markus KRAFT (CAM)

The project aims to develop an automated laboratory of the future using the CARES Laboratory as a demonstration. The primary focus is to create digitised, automated, and interconnected virtual representations of selected laboratory equipment within the CARES Laboratory and to enhance laboratory efficiency by minimising manual paperwork through the digitisation of laboratory operations and experimental processes. Additionally, the project will involve the development of ontologies to describe and document the associated processes, including standard operating procedures. The digitisation and automation of the laboratory is intended to improve quality and compliance by reducing manual errors and variability, and by facilitating data retrieval and analysis. This approach enables faster and more effective problem resolution.

During this reporting period, significant progress was made in the development and deployment of digital infrastructure to support automated laboratory operations. Physical data for various laboratory equipment—such as High-Performance Liquid Chromatography (HPLC), Gas Chromatography–Mass Spectrometry (GC–MS), Thermogravimetric Analysis (TGA), Raman spectroscopy systems, and laser systems—were instantiated in the knowledge graph using developed ontologies.

Ontology development was completed for three modules of a pilot plant located in the CARES laboratory: the chemical dosing module, the chemical reactor module, and the purification module. This work involved extending existing ontologies such as OntoCAPE, OntoDevice, OntoLab, and OntoBMS to represent selected industrial-scale laboratory equipment, including stirred tank reactors, thereby enabling broader applicability beyond traditional laboratory-scale systems.

Furthermore, enhancements were made to *Marie*, an ontology-driven, large language model-based chatbot, to support advanced querying capabilities. The chatbot now enables users to retrieve physical properties of various chemical species—including zeolitic frameworks and metal–organic polyhedra (MOPs)—with high accuracy, thereby facilitating the evaluation of chemical suitability for specific equipment and experimental procedures.

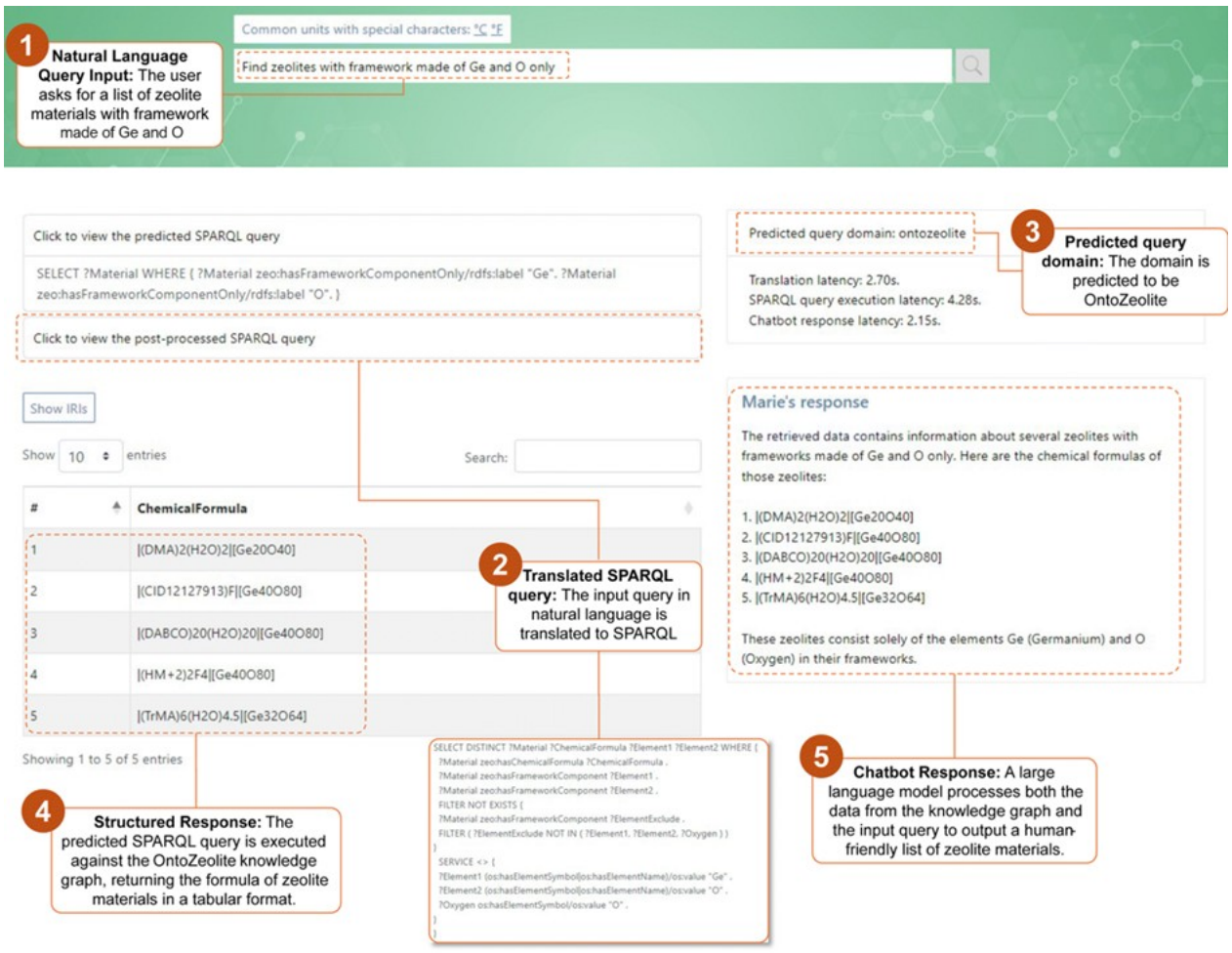


Figure 4.2: User interface of Marie, the ontology-driven and large language model-based chatbot, illustrating the process of querying zeolites and the sequential steps involved in data retrieval.

Scientific output

The following are the CREATE-acknowledged publications generated by the C4T programme during the reporting period, excluding those already featured in the Scientific Highlights section on page 8.

A Platform Ecosystem Providing New Data For The Energy Transition

Markus Duchon, Jessy Matar, Mahsa Faraji Shoyari, Alexander Perzylo, Ingmar Kessler, Patrick Buchenberg, Philipp Kuhn, et al., *ACM SIGEnergy Energy Informatics Review*

DOI: 10.1145/3717413.3717435

Abstract: There is a great need for high-quality and comprehensive data in the energy sector. This data is collected and preprocessed at considerable expense and is not only required for research, but also by planning offices and other industries in connection with planning activities, such as the creation of municipal heat planning. The NEED ecosystem will accelerate these processes establishing an efficient, robust, and scalable energy data ecosystem. Heterogeneous energy-related data sources will be brought together and automatically linked consistently across different sectors as well as temporal and spatial levels. In this context, existing data sources will not be replaced but rather integrated into the NEED ecosystem as dedicated sources including a semantic description on how to utilize them. In addition to conventional data sources from the various planning levels, we envision a quality assessment scheme based on the FAIR criteria. In reality, we are often faced with missing data, too. To close this gap we explore data-driven, model-driven, AI-based, and tool-driven generation of synthetic data. These heterogeneous data sources will be interlinked using ontology modules which will be represented in a knowledge graph. Via a semantic API, queries will be generated to identify the required data sources, which will be orchestrated to provide the data needed. This will enable researchers, planners, and others including their tools to interact with the NEED ecosystem, while a tool proxy will be able to translate the resulting data into proprietary formats, required by some tools to operate. The NEED ecosystem is planned to be a robust, easy-to-maintain, and flexible infrastructure to enhance planning energy measures at different spatial levels and with different time horizons. We envision to evaluate our NEED approach for the transparent provision of data by integrating relevant data sources as microservices, definition and analysis of application scenarios in the planning domain, as well as the integration of various tools for different planning purposes. With these elements, we will be able to quantify the efficiency of data procurement and demonstrate the functionality of the approach using practical use cases.

Simulations of Decane-Ammonia Autoignition in Two Mixture Fractions

Angelos Kylikas and Epaminondas Mastorakos, *Frontiers in Mechanical Engineering*

DOI: 10.3389/fmech.2024.1498820

Abstract: This paper presents a zero-dimensional Doubly Conditional Moment Closure (0D-DCMC) methodology for investigating dual-fuel combustion involving ammonia and diesel. The approach uses two mixture fractions as conditioning variables, one for each fuel, to effectively model ignition and reveal the flame structure in mixture fraction space. Initially, 0D reactor calculations are performed using Cantera, exploring the chemical mechanism, identifying the most reactive mixture fractions, and determining key species involved in the ignition process. Following that, the 0D-DCMC simulations carried out provide understanding into the effects of the scalar and cross-scalar dissipation rates on autoignition. The results show that higher scalar dissipation rates delay ignition, while a negative cross-scalar dissipation rate reduces ignition delay compared to a positive rate. The ignition is shown to occur near the most reactive mixture fraction of the most reactive fuel, at lower conditional values of the less reactive fuel's mixture fraction. The species fronts formed are observed to follow a trajectory between the stoichiometric mixture fractions of the fuels. The results establish a robust computational framework for modeling dual-fuel combustion.

Natural Language Access Point to Digital Metal–Organic Polyhedra Chemistry in The World Avatar

Simon D. Rihm, Dan N. Tran, Aleksandar Kondinski, Laura Pascazio, Fabio Saluz, Xinhong Deng, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *Data-Centric Engineering*

DOI: 10.1017/dce.2025.12

Abstract: Metal–organic polyhedra (MOPs) are discrete, porous metal–organic assemblies known for their wide-ranging applications in separation, drug delivery, and catalysis. As part of The World Avatar (TWA) project—a universal and interoperable knowledge model—we have previously systematized known MOPs and expanded the explorable MOP space with novel targets. Although these data are available via a complex query language, a more user-friendly interface is desirable to enhance accessibility. To address a similar challenge in other chemistry domains, the natural language question-answering system "Marie" has been developed; however, its scalability is limited due to its reliance on supervised fine-tuning, which hinders its adaptability to new knowledge domains. In this article, we introduce an enhanced database of MOPs and a first-of-its-kind question-answering system tailored for MOP chemistry. By augmenting TWA's MOP database with geometry data, we enable the visualization of not just empirically verified MOP structures but also machine-predicted ones. In addition, we renovated Marie's semantic parser to adopt in-context few-shot learning, allowing seamless interaction with TWA's extensive MOP repository. These advancements significantly improve the accessibility and versatility of TWA, marking an important step toward accelerating and automating the development of reticular materials with the aid of digital assistants..

Small-Scale Pyrometallurgical Plant for Recycling Spent Lead Acid Batteries: CFD Analysis of a Submerged Lance Furnace, Environmental and Economic Assessment, and Multiobjective Optimization

Andrés Ortiz, Sebastian López, Alejandro Ríos, Henry Copete, Jethro Akroyd, Sebastian Mosbach, Markus Kraft, and Alejandro Molina, *Journal of Cleaner Production*

DOI: 10.1016/j.jclepro.2025.144654

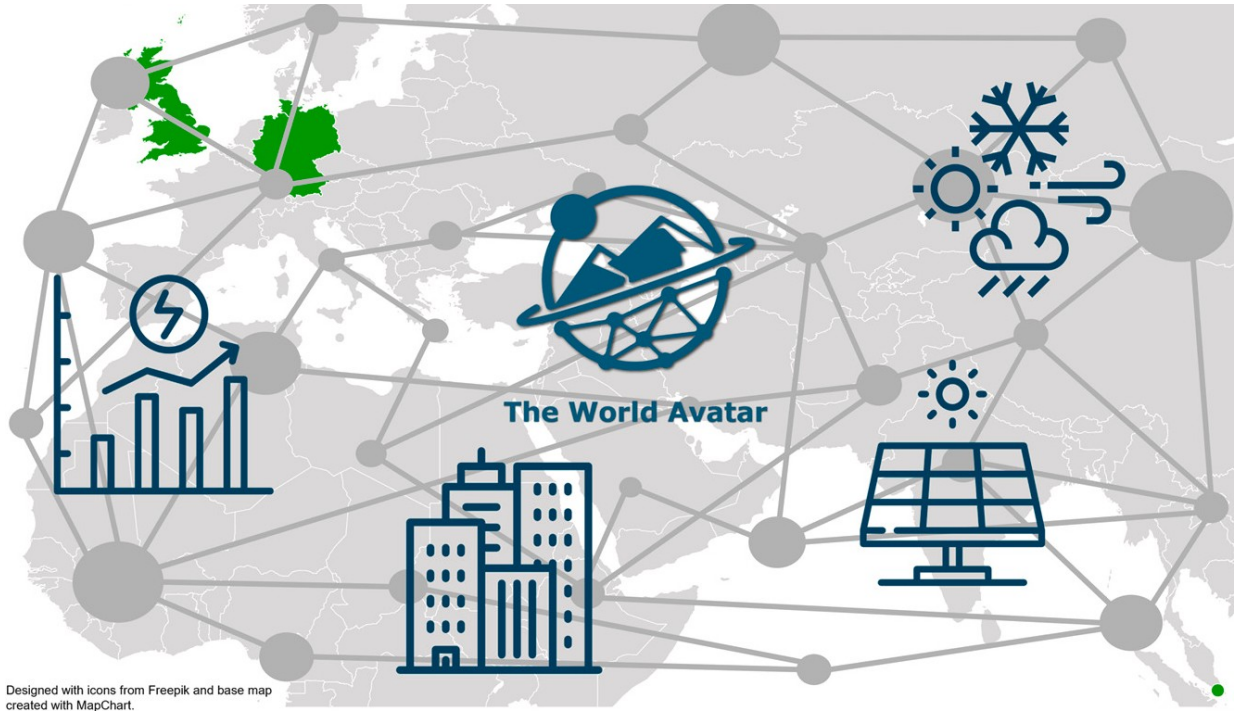
Abstract: A thorough analysis of a small-scale Spent Lead Acid Batteries recycling plant was carried out. The plant included a Top Submerged Lance furnace as a smelter for which a transient model gave insight into the plant operation times and energy requirements. A Computational Fluid Dynamics simulation of the furnace was used to determine the hydrodynamics, thermal efficiency, and to establish a correlation of fuel flow and the smelter temperature. An environmental and economic assessment was conducted based on two indicators: the Environmental Impact Load (EIL) and the Net Present Value (NPV) as computed from the simulation of the pyrometallurgical recycling process in Aspen Plus®. The EIL considered the equivalent CO2, SO2; and 1,4-dichlorobenzene emissions, however the CO2 equivalent emissions were two orders of magnitude higher than those of SO2 and 1,4-dichlorobenzene and dominated the EIL. Six input variables: smelter and refining temperatures, the flow of fluxes (C, Fe2O3, Na2CO3), and water flow were systematically varied in more than 2500 Aspen® simulations to conduct a sensitivity analysis of the effect of the input variables on EIL and NPV. The results indicated that the smelter temperature was, by two orders of magnitude, the most relevant input variable for SLAB recycling in a pyrometallurgical process. The fluxes of carbon and iron (III) oxide had an impact on the process, but on a much lower scale. An optimization of the plant performance based on a function ($f=\alpha EIL EIL+\alpha NPV NPV$) that considered weighting factors for EIL and NPV indicated that the lowest temperature selected for the smelter (1173 K) yielded the lowest values of EIL and the highest NPV. Smelter temperatures below 1173 K were not considered as they would reduce the flowability of the slag. The flow of Fe2O3 had some, but relatively minor impact on NPV. This analysis that applies for the first time a set of simulation tools to address both the environmental and economic impact of a small-scale recycling plant indicated that any efforts devoted to optimize the plant performance in this areas should focus on the reduction of the temperature of the smelter.

Municipal Heat Planning within The World Avatar

Yi-Kai Tsai, Markus Hofmeister, Srishti Ganguly, Kushagar Rustagi, Yong Ren Tan, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *Energy and AI*

DOI: 10.1016/j.egyai.2025.100479

Abstract: This paper presents a novel integration of building energy simulation with The World Avatar (TWA), a dynamic knowledge graph and agent-based framework designed for comprehensive and interoperable digital representation of the world. The study addresses the imperative for accurate and granular building energy data in energy planning scenarios. By leveraging knowledge graph, agents within TWA replace default assumptions in simulation tools with real-time and location-specific input data, such as building geometry, usage, weather, and terrain elevation. This integrated approach automates the simulation process, enabling agents to retrieve input data, execute simulations, and update the knowledge graph with results in a consistent format. To demonstrate this approach, we developed a simulation agent using the City Energy Analyst. Validation against external datasets from Germany and Singapore shows that the agent significantly improves simulation accuracy. The study also highlights the challenges in data acquisition and processing for municipal heat planning, aligning with the requirements of the German Heat Planning Act. Using Pirmasens, a mid-sized city in Germany, as an example, we demonstrate the practical applicability of the agent in municipal heat planning by providing highly granular data on the heating demands and the solar potentials for heat generation. An accompanying economic analysis further evaluates the cost implications and energy storage requirements associated with the installation of solar collectors, and identifies zones in the city with high solar suitability. These insights enable data-driven decision-making, showcasing the potential of this integrated approach to support municipal heat planning.

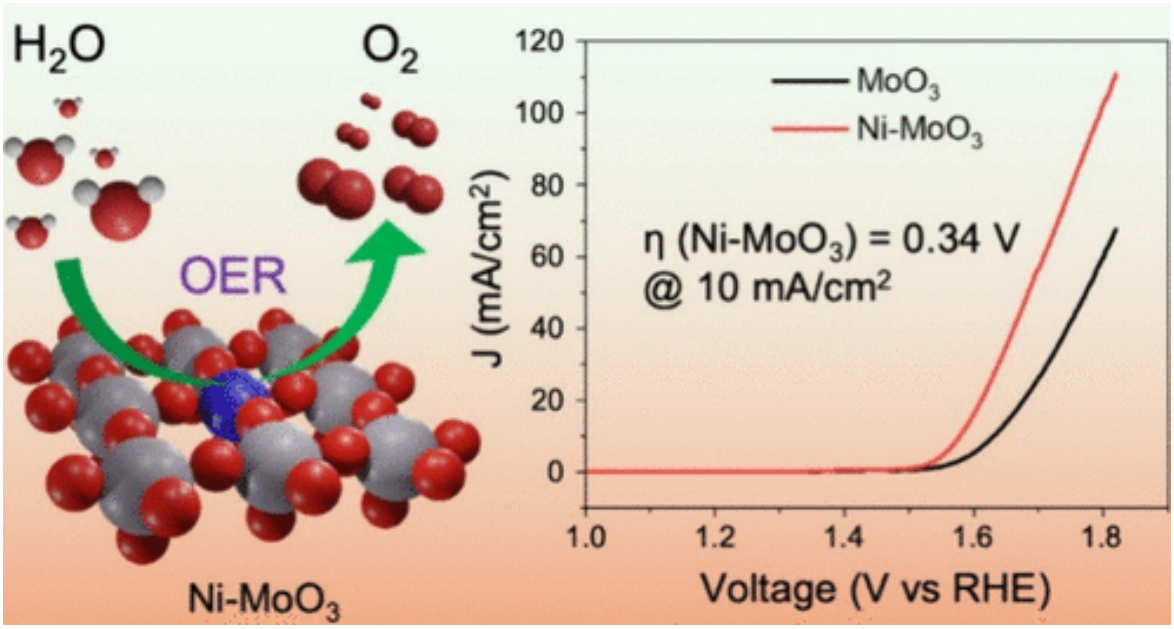


Robust Oxygen Evolution on Ni-Doped MoO3 : Overcoming Activity–Stability Trade-Off in Alkaline Water Splitting

Ankit Kumar Verma, Shahan Atif, Abhisek Padhy, Tej S. Choksi, Prabeer Barpanda, and Ananth Govind Rajan, *Chem & Bio Engineering*

DOI: 10.1021/cbe.4c00160

Abstract: Electrochemical water splitting using earth-abundant materials is crucial for enabling green hydrogen production and energy storage. In recent years, molybdenum trioxide (MoO3), a semiconducting material, has been proposed as a candidate catalyst for the oxygen evolution reaction (OER). Here, we advance nickel (Ni) doping of MoO3 as a strategy to increase the activity and stability of the material during alkaline electrochemical water splitting, thereby overcoming the typical activity-stability trade-off encountered with OER catalysts. The instability of MoO3 in alkaline media can be mitigated by doping with Ni, whose oxide is stable under such conditions. Using density functional theory (DFT) with Hubbard corrections, we show that Ni doping reduces the thermodynamic OER overpotential on the MoO3 basal plane to 0.64 V. Experiments demonstrate that Ni-doped MoO3 requires an overpotential of 0.34 V for an OER current density of 10 mA/cm2 (and 0.56 V at 100 mA/cm2), as opposed to a value of 0.40 V for pure MoO3. Further, Ni-doped MoO3 exhibits a lower Tafel slope of 74.8 mV/dec, compared to 98.3 mV/dec for the pristine material under alkaline conditions. While Mo leaches in alkaline conditions, X-ray photoelectron spectroscopy reveals enhanced stability with Ni doping. Overall, our work advances Ni-doped MoO3 as a promising water-splitting electrocatalyst and provides new insights into its OER mechanism and stability in alkaline media. More generally, the work sheds light on choosing a dopant to increase a material's activity and stability, which will also find applications in other catalytic materials.



Impact of Heat Pumps and Future Energy Prices on Regional Inequalities

Jieyang Xu, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *Advances in Applied Energy*
DOI: 10.1016/j.adapen.2024.100201

Abstract: The adoption of heat pumps to displace the use of gas for domestic heating is a major component of the strategy to reduce emissions in the UK. This study examines the impact of adopting heat pumps on regional inequalities in the UK. An index is used to assess how variations in household fuel costs could affect regional disparities across different future price scenarios. The findings reveal that, at 2019 prices, most households would face higher heating costs with heat pumps. However, following the 2022 energy price shock, heat pump adoption would lead to lower heating costs for most households compared to gas heating. The effect is sensitive to the electricity-to-gas price ratio, with regions experiencing high fuel poverty being most vulnerable to negative impacts. By mapping these geospatial effects, the study enables the forecasting of future inequality trends, providing insights for informed policy development. The results suggest that, under appropriate price structures, heat pump adoption could contribute to both decarbonisation and reduced social inequality. An example mechanism for financial support to mitigate the impact of adopting heat pumps on inequality is demonstrated. This study highlights the novel capability of The World Avatar (TWA) approach to integrate cross-domain data sets, combining energy policy with social equity goals. By forecasting future inequality trends based on energy price scenarios, the study provides a route to valuable insights to support informed policy development, highlighting how the adoption of heat pumps can influence regional inequalities and emphasising the need for targeted interventions to support vulnerable regions.

Ferroelectric Polarization Effects of Single-Atom Catalysts on Water Oxidation

Hao Ma, Xinyu Ye, Xiaoning Li, Zhichuan J. Xu, and Yuanmiao Sun, *Advanced Materials*
DOI: 10.1002/adma.202500285

Abstract: The oxygen evolution reaction (OER) performance of single-atom catalysts (SACs) heavily depends on their substrates. However, heterojunctions with traditional substrate materials often fail to provide the desired dynamic interface effects. Here, through a systematic study of the ferroelectric heterostructure In2Se3/C-N-M, the feasibility of using ferroelectric materials to achieve dynamic optimization of the OER activity on SACs is demonstrated. The ferroelectric In2Se3 is confirmed to be an effective substrate for improving the stability of various SACs, supported by theoretical results of their negative formation energy and positive dissolution potential. Activity analysis indicates that among these In2Se3/C-N-M systems, the In2Se3/C-N-Ir can achieve near-ideal catalytic activities through polarization switching. It can unprecedentedly catalyze OER via a hybrid pathway of adsorbate evolution mechanism and O-O coupling mechanism under different pH conditions (from pH = 1 to pH = 13). Machine learning models have been developed to conduct feature analysis and make ultrafast predictions of OER activity, which identify that the interfacial charge transfer triggered by ferroelectric polarization is the key to fine-tuning the OER performance of SACs. This work provides a theoretical framework that utilizes ferroelectric polarization as a powerful approach to navigate the design of efficient SACs.

Other activities and achievements

Sustainable Reaction Engineering

Ms Xianyue WU (Research Assistant, CARES) is working with Alganaza Pte. Ltd. to run **c**arbon dioxide processing agent (CDPA) tests.

Assoc Prof Wen LIU (Paul) (PI, NTU) was invited by Gates Cambridge to be part of the scholarship panel for interviews being held in Singapore on 28th and 29th March in the CREATE Tower.

Electrochemistry

Dr Qikai SHEN (Research Fellow, NTU) presented "Unravelling Intrinsic Electronic Factors in Thermocatalysis with Electric Polarization" at the Trilateral Conference on Advances in Materials Science in Singapore from 24–26 March 2025.

Dr Chencheng DAI (Research Fellow, NTU) presented a poster during the Singapore Maritime Research Conference 2025.

Dr Dai also delivered an oral presentation titled "Suppressing product crossover and C–C bond cleavage in a glycerol membrane electrode assembly reformer" at the 12th Singapore International Chemical Conference from 9–13 December 2024.

Dr Dai has several technical disclosures:

- An Electrochemical Reformer For Hydrogen Production From Methanol. Other inventors are **Prof Zhichuan Jason XU (PI, NTU)** and **Prof Adrian FISHER (PI, CAM)**. Filed TD Number: 2024-467.
- A Membrane Electrode Assembly Glycerol Reformer to Suppress Product Crossover and C-C Bond Coupled with Energy-efficient Hydrogen Cogeneration. Other inventors are Prof Xu and Prof Fisher. Filed TD Number: 2024-072.
- Ammonia Cracker (previously "An MEA Electrolyzer For Hydrogen Production By Electrochemical Cracking Of Ammonia" merged with "Acid-Alkali Membrane Electrode Assembly Electrolyzer For Hydrogen Production By Ammonia E-Cracking"). Other inventors are Prof Xu, Prof Fisher, and Dr Kamal ELOUARZAKI (Co-Founder of Datumelectronix, C4T spin-off). International Publication Number: WO 2024/237855 A1.

Maritime Decarbonisation

Dr Mutian MA (Research Fellow, CARES), **Dr Li Chin LAW (Research Fellow, CARES),** and **Dr B HARIKRISHNAN (Research Fellow, CARES)** had a shared CARES booth at EXPO@Singapore Maritime Week from 25–27 March 2025 with the digitalisation group and CARES spin-off, 3Y Energy. The larger week-long 2025 event attracted more than 30,000 local and international attendees, including a younger Junior College and Polytechnic-level audience. Dr Law, co-founder of EMICAST, showcased the Voyage Analyser at Singapore Maritime Week 2025 and successfully demonstrated its value in comparing the performance of various low-carbon solutions.

Prof Epaminondas MASTORAKOS (PI, CAM) gave a topical presentation on "Bridging university R&D with the maritime industry" during Singapore Maritime Week 2025 on 26th March 2025. Other speakers included **Prof Christine ROUSSELE (HYCOMBS PI, Université d'Orléans)**, Prof Michael BREAR (University of Melbourne), and Dr Donato ZANGANI (RINA). They shared recent technological developments from university R&D centres and the importance of innovating research together with industry.

EMICAST, the spin-off co-founded by Dr Law and Prof Mastorakos, signed an NDA with Value Maritime in November 2024.

Carbon Policy

Dr J. Lemuel MARTIN (Research Fellow, NTU) was nominated by CARES to attend the Global Young Scientist Summit 2025 (organised by NRF) from 6–10 January 2025.

Digitalisation

- Presented the City Energy Analyst agent under The World Avatar at the CEA User Workshop hosted by the Singapore-ETH Centre from 14–15 October 2024.

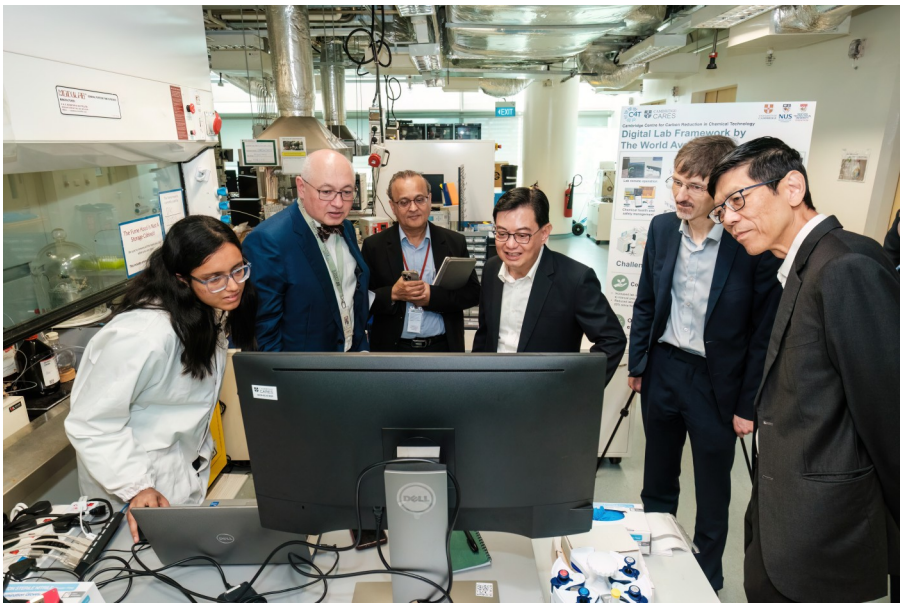
- "Urban Resilience: Shaping Sustainable and Future Ready Cities", as part of the CREATE Seminar series hosted by the Singapore ETH Centre on 6th November 2024.
- **Mr Shin Zert PHUA (Associate Technical Product Manager, CARES)** presented a poster of The World Avatar at the Global Young Scientist Summit 2025 (organised by NRF) on 7th January 2025.

Prof Markus KRAFT (PI, CAM) presented The World Avatar and its applications in various domains, including smart cities and laboratory automation, for the Chairman of NRF and the former Deputy Prime Minister of Singapore (2019–2025), Mr Heng Swee Keat, during his visit to the CARES laboratory on 4th December 2024.

A following *Straits Times* article was written about the visit, "New projects worth $31m to help chemical, energy sectors in Singapore ditch fossil fuels", which included a quote from Prof Kraft, the former Director of CARES (2013–2024).

Photos from Singapore Maritime Wek 2025:

Top left: Prof Epaminondas Mastorakos with Mr Niam Chiang Meng (Chairman, Maritime & Port Authority of Singapore (MPA)) and Mr Loh Khum Yean (Deputy Chairman, MPA); Top right: Dr Mutian Ma and Ms Srishti Ganguly; Bottom left: Dr Li Chin Law; Bottom right: Dr B. Harikrishnan (right).



Photos from Mr Heng Swee Keat's visit in December 2024.

Top: Closed-door discussion; Middle: Mr Heng Swee Keat addresses (from left to right) Prof Sir John Aston, Prof Tan Chorh Chuan, and Prof Alexei Lapkin; Bottom: Ms Srishti Ganguly and Prof Markus Kraft (left) showing Mr Heng Swee Keat the lab digitalisation work.

CLIC

CENTRE FOR LIFELONG LEARNING AND INDIVIDUALISED COGNITION

CLIC is a flagship programme in the Science of Learning initiative to harness advancements in neuroscience to develop training programmes for lifelong flexible learning. The research team has made significant headway since the commencement of the program. Investigators in the four different workgroups have worked continuously and collaboratively to ensure an optimal and cohesive task battery, data collection, organisation, and analysis.

Professor Annabel CHEN Shen-Hsing
Nanyang Technological University

Professor Zoe KOURTZI
University of Cambridge

OVERVIEW

CLIC is committed to advancing lifelong learning and cognitive flexibility through innovative interdisciplinary research, with the goal of developing educationally relevant cognitive flexibility paradigms that inform future interventions across the lifespan.

In January 2025, CLIC officially settled into our new office space in CREATE Tower, marking an exciting new chapter. The new central location makes it an ideal location for engaging with the wider public and the larger facilities fosters an engaging, vibrant, and collaborative environment for the team. The move to CREATE has undeniably placed CLIC in the spotlight. The team was officially included as a CREATE entity during the CREATE Seminar in January 2025. During the event, CLIC Research Fellow Dr Kastoori Kalaivanan delivered an insightful talk on CLIC's studies and findings, attracting an audience of over 100 guests. March was another bustling month for CLIC, with notable events such as hosting the new NRF CEO John Lim, connecting the team with the various CARES entities, and supporting the Gates Cambridge visit to Singapore where Prof Victoria Leong and Prof Henriëtte Hendriks was invited to be part of the scholarship panel for interviews being conducted in Singapore. CLIC also warmly welcomed Prof Hendriks in March as she will be serving her residency with us till June 2025.

Development of the Structure Learning Based Cognitive Flexibility Training Suite (SLiCX) is advancing smoothly, with ongoing collaborations across the various workgroups. The SLiCX Workgroup – a new addition to the CLIC team – was formed to focus specially on developing the SLiCX suite and study protocols. The team has been hard at work setting up cognitive tasks and the main structure-learning intervention on a centralised server and we anticipate that this will be ready in the coming months for the pilot studies. Findings from the pilot will be instrumental in the refinement of the task battery and training protocols for the main study.

Finally, the team is preparing for the upcoming SAC meeting which is expected to take place in mid-2025. As part of this preparation, Phase 1 findings have been thoroughly reviewed, and promising research areas for Phase 2 have been identified. The CLIC consortium has highlighted the impactful work of the Phase 1 studies, ongoing Phase 2 developments, milestones achieved, challenges overcome, and the broader influence CLIC has had within the scientific community and beyond. These developments have been detailed in a report for the SAC, which is now in its final stages of preparation.

Professor Annabel Chen Shen-Hsing
Director of CLIC, NTU

Professor Zoe Kourtzi
Director of CLIC, CAMBRIDGE

Update on Phase 1: Neuroimaging Data Analysis

Dr Deepika SHUKLA (Research Fellow, NTU) expanded analysis of the MR spectroscopy (MRS) data in Phase 1 to investigate the impact of hemispheric lateralisation on the behavioural measures associated with training from the Structure Learning (SL) and cognitive flexibility (CF) tasks. This research was showcased as a poster at the Annual Meeting of the Society for Psychophysiological Research (SPR) in October 2024. Findings revealed that SL training leads to metabolic modulation that affects both hemispheres, enhancing the performance of the Training group, indicating an improved cognitive flexibility in the CST task. Dr Shukla and **Dr Eleanor KOO (Research Fellow, NTU)** met with Cambridge Research Fellows to review Phase 1's data processing and analysis methods. Dr Shukla revised the MRS data analysis pipeline to assess GABA and Glutamate as measured variables rather than GABA+ (GABA + macromolecules) and Glx (Glutamate + Glutamine), as this method provides provided a better relationship with the neuronal inhibition/excitation (I/E) balance.

The analysis of Multiparametric mapping (MPM) data has been updated to evaluate ROI specific changes in Gray and White matter separately. With assistance from **Dr Ke TONG (Research Fellow, NTU)**, CF metrics from the data were integrated into composite variables as CF1 (set-shifting flexibility) and CF2 (strategy flexibility) scores. Multimodal data analysis of MRS and MPM measurands from the bilateral dorso-lateral pre-frontal cortex (DLPFC) were correlated with the SL strategy (mean ICD) as well as CF1 and CF2 scores. A significant correlation was observed between changes in the bilateral I/E balance and the SL strategy, while only the right DLPFC I/E balance related to CF2 in the training

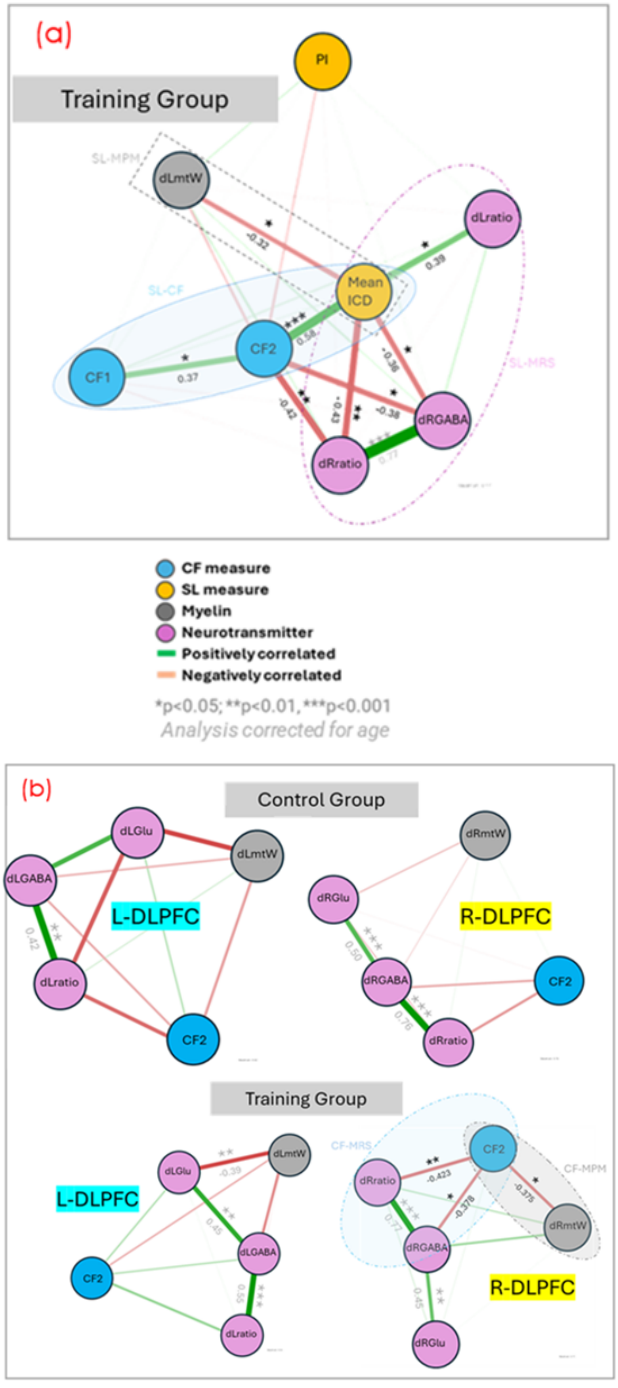


Figure 5.1: Multimodal neuroimaging and behavioural data analysis. (a) Partial correlation of neuroimaging measures with SL and CF scores in the SL intervention group. (b) Partial correlation of bilateral DLPFC neuroimaging measures with CF2 (strategy flexibility scores) in the control and SL training groups.

group, with no neuroimaging measures correlating with CF1. Furthermore, these relationships were specific to the SL intervention group and were not seen in the control group (Figure 5.1). A portion of this work has been submitted and accepted for oral and poster presentations at the upcoming Organisation for Human Brain Mapping (OHBM) annual meeting in Brisbane, Australia in June 2025.

While progress on the rs-fMRI data analysis has slowed following Dr Koo's departure, the team has begun reprocessing the data and are optimistic about obtaining results in the next quarter.

Update on Phase 2: Work Package 1

Preparations for Data Collection

A dedicated team was formed to focus on the development of the Structure Learning-based Cognitive Flexibility Training Suite (SLiCX). This team is led by **Dr Kastoori KALAIVANAN (Research Fellow, NTU)**, who is primarily responsible for conceptualising and executing the SLiCX adult and adolescent pilot studies. Together with **Prof Annabel CHEN (Director and PI, NTU),** Dr Kalaivanan leads the team in preparing for the upcoming Phase 2 studies. The team has designed three pilot studies to test the salience of an additional dimension (i.e. shapes) to enhance task complexity and the different training contingencies. The first pilot study has received IRB approval and is ready to start in May 2025. Dr Kalaivanan also leads the manuscript preparation on developing an abbreviated version of the verbal fluency task in the SLiCX team. The team has also met with creators of the game "All you Can E.T." from the NYU-CREATE lab (PI: Professor Jan Plass) and are currently exploring protocols to deploy this task on the CLIC server.

Cognition and Infancy Studies

Dr Xinchen FU (Research Fellow, NTU) is working on data analysis for the CLIC infancy projects, with a focus on exploratory behaviour and the role of social context in early cognitive development. She leads the EEG preprocessing and analysis, including eye-blink component extraction and dynamic functional connectivity (dFC) modelling, to support the integration of neural and behavioural indices of explore–exploit strategies. Dr Fu also coordinates data collection and tasks development for Phase 2 of the infant study, which examines the developmental links between creativity and executive function (EF). In the CLIC infancy project, **Dr Ke TONG (Research Fellow, NTU)** modelled the temporal patterns of infant exploratory behaviours across different social contexts, enhancing our understanding of early cognitive flexibility and creativity development. Dr Tong He also works on the development of SLiCX training suite for the Phase 2 studies. In January, Dr Tong presented CLIC research in the Science of Learning session with other CRADLE and NIE researchers during the MOE Academic Research Council (ARC) visit to NTU.

Mr Timurcan OZCELIK (Research Assistant, NTU) leads the development and piloting of a novel creative problem-solving task designed for toddlers aged 2–3 years, contributing to methodological innovation in the CLIC Phase 2 infancy projects. He coordinated participant recruitment and outreach, led experimental piloting, and refined testing protocols to ensure age-appropriateness and data quality. Mr Ozcelik also contributed to manuscript preparation, focusing on the development of novel analytical approaches to quantify cognitive flexibility and creativity. These include explore–exploit metrics, shifting strategies in sequential categorisation behaviour, and complexity-based measures as alternative indicators of early creative potential.

Mr Angshuk DUTTA (Research Assistant, NTU) has worked on establishing technical protocols for data collection and computational analyses of the Remote Associates Test (RAT) and Verbal Fluency (VF) datasets. In collaboration with Dr Tong, Mr Dutta leveraged large language models (LLMs) to derive shared semantic representations for every VF corpus word and tracked how these representations evolved. As the geometry of these embeddings depends strongly on model architecture and training regimen, he systematically benchmarked multiple state of the art LLMs to identify those offering the most robust—and therefore most informative—semantic spaces for downstream linguistic analyses.

Neuroimaging

In preparation for Phase 2 of the study's neuroimaging pilot, **Dr Deepika SHUKLA (Research Fellow, NTU)** has collaborated closely with the radiography team at Cognitive Neuroimaging Centre (CoNiC) at NTU to modify the neuroimaging protocol from Phase 1 and integrate the scanner SL task administration, along with additional diffusion imaging sequence.

Development of Neuroimaging Pilots

The Neuroimaging team along with **Dr Eleanor KOO (Research Fellow, NTU)** planned a neuroimaging pilot study for Phase 2 that includes both Adults and Adolescents, employing a pre- and post-test design. The existing Magnetic Resonance Imaging (MRI) data collection protocol has been adapted from the neuroimaging protocol in Phase 1 and incorporates a structure learning (SL) task within the scanner, where participants engage in an SL game while the MRI scans occur simultaneously. Participants' responses are recorded using a 4-button box to evaluate their performance and accuracy during the task. The revised protocol features additional Diffusion Spectrum Imaging to capture changes in structural connectivity induced by training. **Mr Wei Ler KOO (Research Assistant, NTU)** oversees the coordination with CoNiC to secure MRI scanner bookings. **Ms Winlynn CHOO (Research Associate, NTU)** assists with laptop maintenance and video editing for materials used during the MRI sessions. **Ms Tanisha ATTRI (Research Assistant, NTU)** ensures participant readiness and supports Dr Shukla during imaging sessions by presenting the SL task and facilitating both verbal and non-verbal communication throughout the imaging process. With Ms Attri's assistance, the IRB application for the initial neuroimaging pilot and an amendment to include new staff have been submitted and approved. The team has piloted the modified MRI protocol for Phase 2 and collected data from two participants in both the Adult and Adolescent groups. Recruitment is still ongoing, and the team aims to have the pilots completed by July 2025.

Data Quality Check and Analysis

The team introduced an instructional presentation and nature visual to be played in-scanner along with multiple verbal and non-verbal checks, to ensure a better experience for both adult and adolescent participants and improve the overall imaging protocol for this phase. As an initial measure for quality control in neuroimaging, Dr Shukla conducted quality assessments and data processing following data collection. Meanwhile, both Ms Attri and **Mr Gabriel ANG (Research Assistant, NTU)** are engaging in a literature review and exploring a potential preprocessing pipeline for functional and diffusion data that can be implemented as a standardised workflow in future data processing efforts.

Update on Phase 2: Work Package 2

Dr Nadhilla Velda MELIA (Research Fellow, NTU) has been leading the team on study preparations and data collection for the language learning intervention study among young adults, which is currently in its pilot stage. Under the supervision of **Prof Henriëtte HENDRIKS (Deputy Director and PI, CAM)**, who is in Singapore for her residency, Dr Melia and the team are running the post-test in the Modern Languages Centre of NTU in April with 30 student participants. The main three-arm study with young adults is planned for the start of the new academic year (2025-26) and will also involve students from the Language and Communication Centre and students in the Business school. Connections with the Institute of Adult Learning are being set up to pursue the study with working adults with help of **Prof Annabel CHEN (Director and PI, NTU)**. The language interventions will allow the team to measure the advantages of learning a second language on executive functions and in particular, cognitive flexibility within learners. Dr Melia has also been preparing manuscripts for publication, relating to social factors, particularly multilingualism, with Prof Hendriks. They are both currently working on three manuscripts: 1) "Validation of the CILD-Q for Measuring Multilingualism in Singapore" (Melia et al., under revision), 2) "The Relationship between Multilingualism and Perceived Social Support" (Melia et al., in preparation), and 3) "Multilingualism and Cognitive Flexibility" (Melia et al., in preparation).

Prof Hendriks is also part of the discussions on a paper, being prepared by **Dr Shengchuang FENG (Research Fellow, NTU)**, on cooperativeness and the use of language in Singapore, and the validation of the CILD-Q questionnaire in the adolescent population with the School team. Dr Feng has been working on three manuscripts: (1) "QualGames: A database and a Qualtrics implementation of behavioural game theory tasks" (Feng et al., under revision), (2) "Overlooked for three decades: A systematic examination of a problematic item in the 10-item Big Five Inventory" (Feng et al., in preparation), and (3) "The relationship between language entropy and cooperativeness" (Feng et al., in preparation). Additionally, he is analysing data on the relationship between perceived relative deprivation and sleep quality and is preparing a manuscript based on these findings. He also leads the design of the social framing study in WP2.

In March 2025, **Ms Yoke Loo Emma SAM (PhD Student - IGPCRADLE, NTU)** submitted her doctoral dissertation and successfully defended

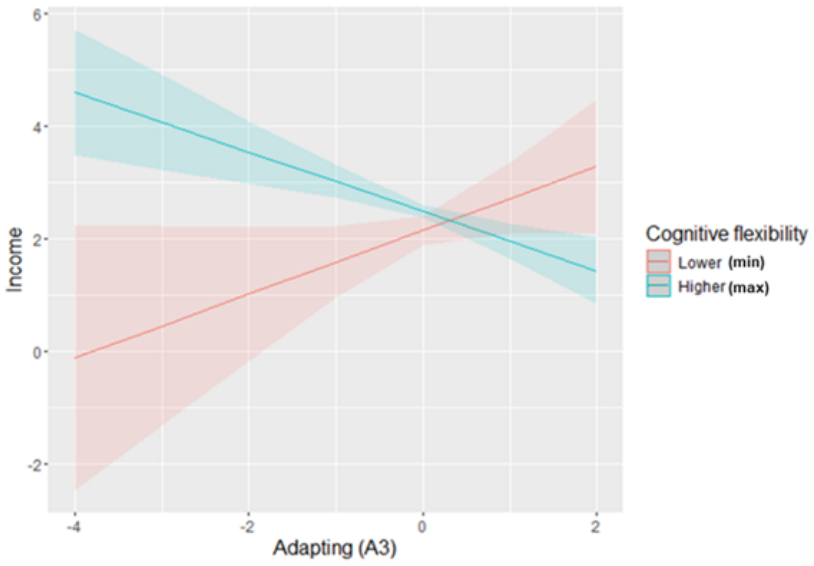


Figure 5.2: The figure shows that adapting behaviour helped individuals with lower cognitive flexibility achieve better outcomes. This finding suggests that individuals with lower cognitive flexibility may benefit from targeted strategies and action plans that strengthen their ability to adapt and overcome career-related challenges.

her thesis, which used data collected in the CLIC project. Her thesis examined how key cognitive functions—particularly cognitive flexibility—relate to practical outcomes such as income and academic achievement among Singaporean working professionals and university students. Key findings highlight the importance of enhancing cognitive flexibility alongside career adaptability to improve career outcomes. For instance, lower cognitive flexibility may be mitigated by proactive career behaviours, such as engaging in job exploration and training to navigate the changing work landscape, thereby supporting better income outcomes. These findings suggest the need for tailored interventions and early educational programmes that integrate cognitive and career adaptability training to strengthen resilience and support career transitions.

Mr Akshay ABRAHAM (Research Associate, NTU) co-leads the Language learning Intervention pilot study while **Ms Yuan Ni CHAN (Research Assistant, NTU)** assists with the general logistics and administrative duties of the team. Ms Chan is currently working on a paper studying the relationship between Trust, Receptiveness to Opposing Views, and Social Value Orientation. **Ms Hui Shan YAP (Research Associate, NTU)** contributes to the logistics, administrative and budget planning for the WP2 studies. Ms Yap is also helping to coordinate and is involved in the planning of measures and execution of the SLiCX study for social related measures.

Update on Phase 2: Work Package 3

The School Workgroup has continued to work closely with the Singapore Examination and Assessment Board (SEAB) on the Critical, Analytical, and Inventive Thinking (CAIT) project. Following the two rounds of data collection which was completed in July and October 2024, the team is planning for further data collection at four local secondary schools scheduled in May 2025. The partnership is key to understanding how critical and adaptive thinking amongst students are related to CF in an academic setting. **Dr Kastoori KALAIVANAN (Research Fellow, NTU)** has been heavily involved in the Crossing Valley project (an innovative bridge construction game) and she helps in facilitating the data collection in collaboration with SEAB. She also leads the manuscript on validating the CILD-Q in Singaporean adolescents.

Dr Rui WANG (Research Fellow, NTU) joined the School Team in March 2025, where she is responsible for preparing data collection (including test program development), analysing Phase 1 data, and general data screening to identify potential relationships in the data. Dr Wang is also working on preparing a manuscript on the relationship between cognitive flexibility and academic achievement. Additionally, Dr Wang provides training for other research associates and assistants within the team.

Ms Joyce CHEUNG (Research Associate, NTU) and **Ms Selvira MELIA (Research Assistant, NTU)** joined the team in March 2025 and are working with Dr Kalaivanan and Dr Wang on preparing manuscript drafts. Both Ms Cheung and Ms Melia are also responsible for coordinating student research assistants and preparing the logistics for the upcoming data collection in May 2025 with NIE and SEAB, which is led by **Dr Nastassja LOPES FISCHER (Research Scientist, NIE). Mr Amos Joshua OH (Research Associate, NTU)** joined CLIC in January 2025 and has been instrumental in driving forward multiple key research initiatives, including SLiCX and school-based studies. His work spans areas like study design, data analysis, and ethics management, alongside project logistics and coordination across the various teams.

CLIC Data Computing Server, Resource Monitoring and Data Transfer Infrastructure

A server migration was conducted in December 2024 with the support of the High-Performance Computing Centre (HPCC) team at NTU to support the needs of secure, large-scale, computer and data intensive computation for CLIC researchers. The CLIC server migration and CLIC data storage is overseen by CLIC's research engineer, **Dr Sheng Hung CHUNG (Research Engineer, NTU).**

All four CLIC servers (Dell PowerEdge R740, R740, R750 and R750) have been migrated to HPCC, North Spine (Blk NS4-04-25) at NTU with enhanced login security for CLIC researchers. Within the HPCC hosting environment, the CLIC server cluster is deployed in a cluster setting and computing nodes integration provides users with high computing availability and distributed workload. CLIC researchers will be given access to the login node: 172.21.2x.4x to interact with the server cluster (e.g. submitting jobs, accessing files) and perform computation and analysis.

Other activities and achievements

Dr Deepika SHUKLA (Research Fellow, NTU) presented a poster on behalf of CLIC titled, "Bilateral Hemispheric Interplay with Adaptive GABA and Glx Modulation Supports Effective Structure Learning" at the 64th Annual Meeting of the Society for Psychophysiological Research (SPR), in Prague, Czech Republic from 23–26 October.

Prof Victoria LEONG (Deputy Director and PI, NTU) and **Prof Henriëtte HENDRIKS (Deputy Director and PI, CAM)** were invited by Gates Cambridge to be part of the scholarship panel for interviews being held in Singapore on 28th and 29th March in the CREATE Tower.

Pictured are Prof Leong and Prof Hendriks (back left) attending the Gates Appreciation dinner in Singapore for the interview panellists.

Scientific output

The following are the CREATE-acknowledged publications generated by the CLIC programme during the reporting period, excluding those already featured in the Scientific Highlights section on page 8.

[Ms Yoke Loo Emma SAM's PhD thesis] Socio-cognitive aspects of career transition

DOI: 10.32657/10356/184212

Abstract: Career adaptability – a crucial contemporary meta-competency for navigating career changes and challenges – is vital in today's rapidly evolving work environment. The Career Construction Model of Adaptation (CCMA) by Savickas and Porfeli (2012) provides a comprehensive framework for understanding how individuals manage their career paths. The CCMA emphasises the lifelong process of career construction, highlighting how personal characteristics, skills, and actions interact to influence successful career outcomes. The model is based on four key dimensions – adaptivity, adaptability, adapting, and adaptation, known as the "four As" – to examine the interrelationships between traits of flexibility (adaptivity), self-regulatory resources (adaptability), career behaviours (adapting), and outcomes (adaptation). Each dimension is further broken down into multiple subcomponents, ensuring the model's flexibility and comprehensiveness. Despite its wide adoption in existing studies, the CCMA lacks a comprehensive measurement approach to fully capture the career construction process. Studies examining the serial relationships between its four dimensions often rely on a limited selection of constructs to represent each dimension. For example, individual studies may include only one or two constructs per dimension, which can fail to encompass the framework's multifaceted nature. Moreover, the variation in the choice of measures across studies leads to inconsistencies in how the dimensions are operationalised and interpreted, further limiting the comparability and generalizability of findings. Similarly, while the theoretical concept of CCMA highlights cognitive flexibility (CF) as a core executive function, alongside working memory (WM) and inhibitory control (IC), responsible for managing uncertainties in dynamic environments, most existing research relies on self-reported measures of CF. Although these self-reports are useful for capturing individuals' perceived abilities and willingness to adapt or embrace change, they overlook the underlying cognitive processes, such as the ability to shift attention between tasks or mental models. These processes, which are critical to CF, are better assessed using established cognitive tasks that offer a more objective and comprehensive evaluation of this construct. Three studies were conducted to 1) evaluate the underlying dimensions of the "four As" and their associations within the CCMA framework, 2) examine how CF influences the relationship between the "four As" and income among Singaporean working adults, and 3) assess the impact of CF on the relationship between the "four As" and academic achievement in Singaporean university students. To the author's best knowledge, these questions have not been explored extensively in prior research. Study 1 confirmed the validity of the "four As" by extracting four common factors from diverse measures across samples and validating the serial mediation relationship in working professionals, thereby supporting the theoretical foundation of the CCMA. Study 2 revealed a positive relationship between CF and income. In addition, individuals with higher CF benefited more from improvements in adaptivity (e.g., enhancing one's willingness to be proactive in career development), while those with lower CF gained more from focusing on adapting behaviours, such as engaging in job exploration and training. Study 3 found no significant association between CF and academic performance, although a positive relationship between WM and academic performance emerged. Specifically, higher adaptation scores were associated with better cumulative grade point average (CGPA) for students with lower WM, suggesting that career adapta-

tion – such as beliefs in one's employability, and having a clearer vocational identity – can help to mitigate the adverse effects of lower WM on academic performance. Overall, this thesis offers new insights into the career construction process by systematically evaluating the CCMA framework in two distinct populations, namely working professionals and university students. This is the first comprehensive effort to assess the CCMA, combining psychometric validation and exploring the relationships between cognitive functions and important real-life outcomes. This thesis leverages a multidisciplinary approach by incorporating cognitive science theories (i.e., the concepts of the core triad of executive functions) and methodologies (i.e., task-based cognitive functions metrics) alongside conventional organisational behavioural approaches using well-validated career framework and assessment instruments. These findings can inform individuals, organisations, and policymakers about the benefits of flexible thinking and career adaptability, contributing to training curricula that better prepare the future workforce for the ever-changing economy.

HYCOMBS

HYDROGEN AND AMMONIA COMBUSTION IN SINGAPORE

HYCOMBS focuses on the combustion fundamentals of hydrogen, ammonia, their blends, and their blends with hydrocarbon fuels. The knowledge acquired in this project will enable the penetration of zero-carbon fuels in the Singapore energy system and this will benefit Singaporean industries and residents.

HYCOMBS leads:

Professor Epaminondas MASTORAKOS
University of Cambridge

Assoc Professor Fei DUAN
Nanyang Technological University

Professor Kaoru MARUTA
Tohoku University

The past six months have seen significant progress in the HYCOMBS project. The project aims to discover knowledge of relevance to the development of NH_3 and H_2 reciprocating engines and gas turbines and to channel this knowledge into useful tools and models to be used in engineering practice.

On the computational front, the modelling software is being developed and validated for NH_3 and H_2 flames and detonations. The chemical mechanism for NH_3/H_2 has been validated against measured data from shock tubes and rapid compression machine from the literature. Meanwhile, the hiring process for a research fellow is ongoing. Once a suitable candidate has been identified, work can commence on modelling related to NH_3/H_2 leaks and detonations.

Currently, the work packages are setting up their rigs for upcoming experimental work. The micro-flow reactor rig is under development, with the planning stage focusing on part design and GC system procurement to measure chemical species such as H_2, N_2O, O_2, Ar, N_2, CO, CO_2 hydrocarbons up to C2 and NH_3. These experiments will address the current uncertainties in the chemical kinetics of NH_3 and H_2 combustion at low to medium temperatures. Figure 6.1 shows the planned experimental setup for the micro-flow reactor rig currently in development.

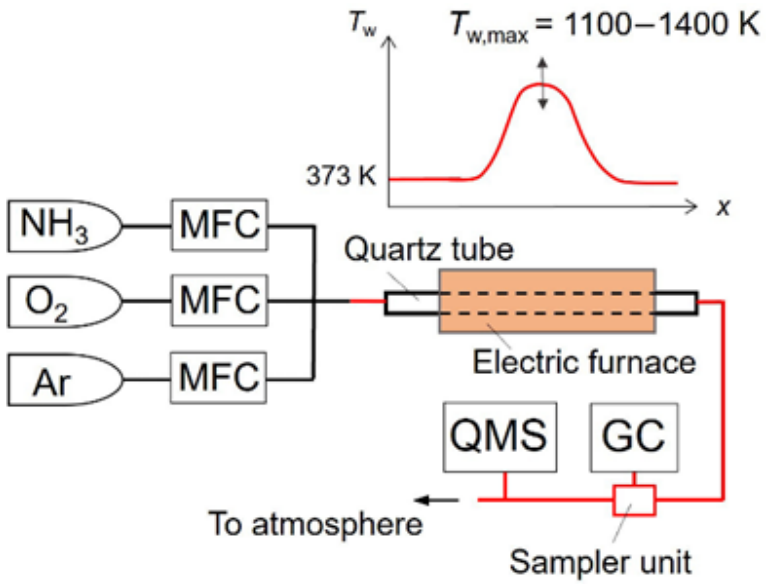


Figure 6.1: Schematic of the planned micro-flow reactor rig. The anticipated wall temperature profile (Tw) of the reactor is as shown in the figure. GC: gas chromatography system; MFC: mass flow; controller QMS: quadrupole mass spectrometer.

A Bunsen burner is under construction to gain a fundamental understanding of combustion instability and pollutant formation in NH_3/H_2 flames. This study will leverage the controlled canonical experimental conditions of the Bunsen burner. The first step is to stabilise and characterise steady flames using complementary optical diagnostics, including spontaneous emission of radicals (OH*, NH*), laser absorption spectroscopy of several stable species (NH_3, H_2O, N_2O), and OH laser-induced fluorescence. This phase will provide an opportunity to develop and validate these diagnostics on ammonia/hydrogen flames, offering novel and valuable insights from both scientific and practical perspectives.

An axially staged swirl burner will be used to investigate flame stability and thermoacoustics, with rig design work and the specification and purchase of acoustic and optical diagnostic systems currently underway. Precision pressure transducers and photomultiplier tubes will be used to characterise the unsteady pressure and chemiluminescence emissions, permitting the characterisation of the thermoacoustic state of the system during NH_3/H_2 operation. The axially staged system is being designed to enable a high degree of flexibility in operating conditions, allowing new staging strategies to be investigated and their effect on thermoacoustic stability to be assessed.

Additionally, a new rig equipped with a turbulent swirl burner is under construction at the CARES lab. This setup enables the investigation of various combustion modes, such as fully premixed, partially premixed, non-premixed, and sequential combustion of NH_3 and H_2. It also allows for the study of different injection strategies, including staged fuel injection and multi-hole injection. These aspects are crucial as swirl-induced recirculation is pivotal for stabilising flames in gas turbines and serves as the first stage in conventional Rich-Quench-Lean systems. The findings will offer valuable insights into the fundamental stability of staged systems operating with H_2 and/or NH_3 and provide baseline cases for simulation validation. Currently, the main components of the burner have been constructed, and additional machining is required to complete the rig assembly.

A high-pressure optical cell is currently in the design phase. It will feature a closed-volume combustion chamber designed to operate at high pressures, simulating the conditions found during the top dead centre of reciprocating engine combustion. The experimental program will utilise a variety of fuel mixtures, including pure NH_3, NH_3/ H_2 blends, pure H_2, and hydrocarbon/ NH_3 blends. These experiments will yield detailed data on the combustion characteristics of these fuels, which will then be supported and complemented by quantitative computational models. This integrated approach aims to provide a deeper understanding of the reaction mechanisms involved in H_2 and NH_3 combustion. Figure 6.2 shows the preliminary design of the optical cell. This design will serve as a foundation and will be subjected to further adjustments and modifications as needed based on ongoing research and development.

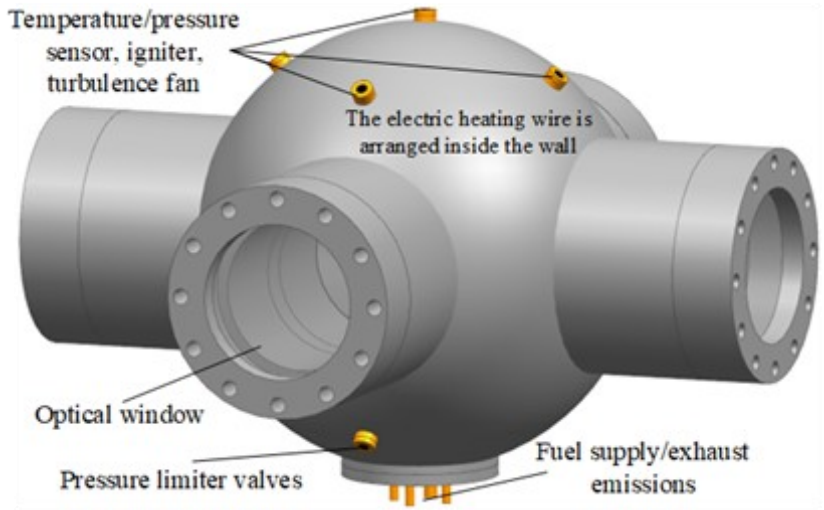


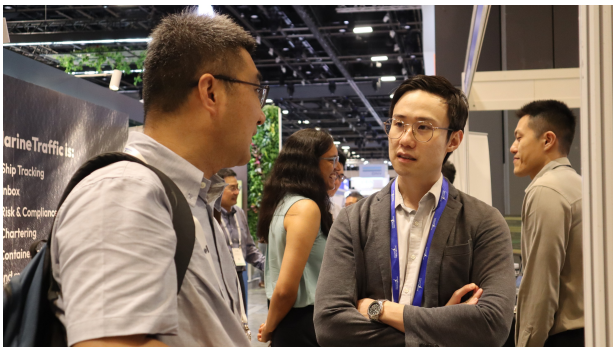
Figure 6.2: Preliminary design of the high-pressure optical cell.

Other activities and achievements

Prof Epaminondas MASTORAKOS (Programme Lead, CAM) and **Prof Christine ROUSSELLE (PI, Université d'Orléans)** gave a topical presentation on "Bridging university R&D with the maritime industry" during Singapore Maritime Week 2025 on 26th March 2025. They shared recent technological developments from university R&D centres at the University of Cambridge and Université d'Orléans in the maritime space. Other speakers included Prof Michael BREAR (University of Melbourne) and Dr Donato ZANGANI (RINA).

Prof Mastorakos and several HYCOMBS researchers showcased the project at the CARES booth during Singapore Maritime Week 2025, facilitating knowledge exchange with industry stakeholders, policymakers, and academic experts.

In December 2024, the Chairman of NRF and the former Deputy Prime Minister of Singapore (2019 –2025), Mr Heng Swee Keat, had a formal discussion with HYCOMBS and SM_3 leads and visited the CARES laboratory. Prof Mastorakos highlighted the project's decarbonisation efforts and new international collaborations with Japanese, French, and Norwegian universities. A follow-up *Straits Times* article, "New projects worth $31m to help chemical, energy sectors in Singapore ditch fossil fuels", was written and included a quote from **Dr Yong Ren TAN (Research Fellow (Project Manager), CARES)**.



Top: Prof Mastorakos, Prof Rousselle, Prof Brear, and Dr Zangani hosting their presentation at Singapore Maritime Week 2025; Middle and Bottom: Dr Tan at the event and the overall CARES booth.

Left: (From left to right) Prof Markus Kraft, Prof Sir John Aston, Prof Mastorakos, Assoc Prof Fei Duan, and Dr Huangwei Zhang at the discussion with Mr Heng Swee Keat; Right: Mr Heng Swee Keat looks at the laser diagnostics instrument that will be used in HYCOMBS.

SUSTAINABLE MANUFACTURE OF MOLECULES AND MATERIALS IN SINGAPORE

SM_3 will aim to shift the chemical manufacturing industry to a more circular, sustainable, and resilient model. This project will address systemic challenges, including the integration of regionally available resources and the development of scalable, flexible technologies for local manufacturing.

SM_3 leads:

Professor Alexei LAPKIN

University of Cambridge

Professor Shunsuke CHIBA

Nanyang Technological University

Professor Ning YAN

Assoc Professor Ming Joo KOH

National University of Singapore

SM_3 is aiming to design a new ecosystem of molecules and technologies that are demonstrably 'net zero'. Specifically this translates into four global objectives:

O1. Identify key 'hub' molecules that can be accessed from 'net-zero' resources and form the backbone of the new 'eco-system' of sustainable manufacture of performance molecules.

O2. Develop new synthetic methods for efficient transformations of 'hub' molecules into performance chemicals.

O3. Develop new synthetic technologies that allow easy scalability and support advanced new synthetic methods.

O4. Identify and develop a sufficient set of process technologies for sustainable manufacture of molecules, using principles of resilience, integration with renewable and waste energy streams and supporting new business models (regional, manufacture on demand, dynamic operation, etc).

To date, the project teams have been heavily engaged in recruitment and identification of specific equipment to purchase. NTU will be hosting the high-throughput synthesis post-docs and their associated equipment.

Thus far, **Dr Raudah LAZIM (Senior Research Fellow, CARES)** has been a recent hire under the supervision of **Prof Alexei LAPKIN (Programme Lead, CAM)**. The project will soon complete hub molecules search and start link prediction work, and start model generation for the initial set of technologies and processes.

Other activities and achievements

In December 2024, the Chairman of NRF and the former Deputy Prime Minister of Singapore (2019 –2025), Mr Heng Swee Keat, had a formal discussion with HYCOMBS and SM_3 leads and visited the CARES laboratory. **Prof Alexei LAPKIN (Programme Lead, CAM)** highlighted the project's decarbonisation efforts and the importance of Singapore as a hub for manufacturing ideas and innovation. A follow-up *Straits Times* article, "New projects worth $31m to help chemical, energy sectors in Singapore ditch fossil fuels", was written about the visit.

Chemical Data Intelligence (CDI), a CARES spin-off, will sponsor a PhD student to join SM_3 via the Cambridge-CARES Studentship scheme and provide expertise in AI for chemistry to the project. CDI will create a dry lab environment for SM_3 to provide a single environment for all post-docs to work on models and for data storage.

Cover image of SM_3: Mr Heng Swee Keat looks at the robot made in the PIPS programme that uses elements of machine learning to improve pharmaceutical manufacturing. SM_3 will leverage similar techniques to create a more sustainable chemical industry model. Left: Prof Alexei Lapkin sits with the British High Commissioner to Singapore, His Excellency Nikesh Mehta, during the formal discussion with Mr Heng Swee Keat.

HD_4

HEALTH-DRIVEN DESIGN FOR CITIES

HD_4 is a groundbreaking research collaboration in Singapore bringing together a world-class team from Singapore and Cambridge. HD_4 will investigate how the urban and social environment exposes people to different risks, and how this influences our behaviour and health. HD_4 will exploit a unique opportunity to work synergistically with the SG100K cohort study, helping us understand how we might change the fabric and organisation of cities to make them healthier for all of us. HD_4 will use an established co-creation approach to work with government agencies to ensure that the tools and public health models that it develops are influential in translating research into action.

HD_4 leadership team:

Professor Nick WAREHAM
University of Cambridge

Professor John CHAMBERS
Nanyang Technological University

Professor Rudi STOUFFS
National University of Singapore

Dr Ronita BARDHAN
University of Cambridge

With cities expanding rapidly around the world, people face growing challenges to their health and wellbeing. Heat, noise, air pollution, and limited opportunities to eat healthily and be physically active. It's time to rethink how cities can support our health.

HD_4 is motivated by the rising burden of non-communicable diseases on individuals and the wider society in Singapore. Alongside efforts to reorganise the healthcare system and improve the efficiency and effectiveness of healthcare through research aimed at personalised prevention, there is a need to develop a complementary approach to realise the vision of improving population health through small changes in large numbers of people. Although this principle underpins the current public health approach, the evidence base that informs interventions is relatively weak. HD_4 will strengthen this evidence base, studying the relationship between the environment, health behaviours and health outcomes. As a nation with ambitious health goals, rich data, and the drive to turn research into real change, Singapore offers a unique setting for this work. HD_4 will work in partnership with government agencies and policymakers to identify opportunities for change, so that the science can guide Singapore's planning and health strategies in the years ahead.

HD_4 is being operationalised in two phases. The critical contribution of the current phase – Phase 1 – will be to demonstrate the **feasibility** and **necessity** of the research.

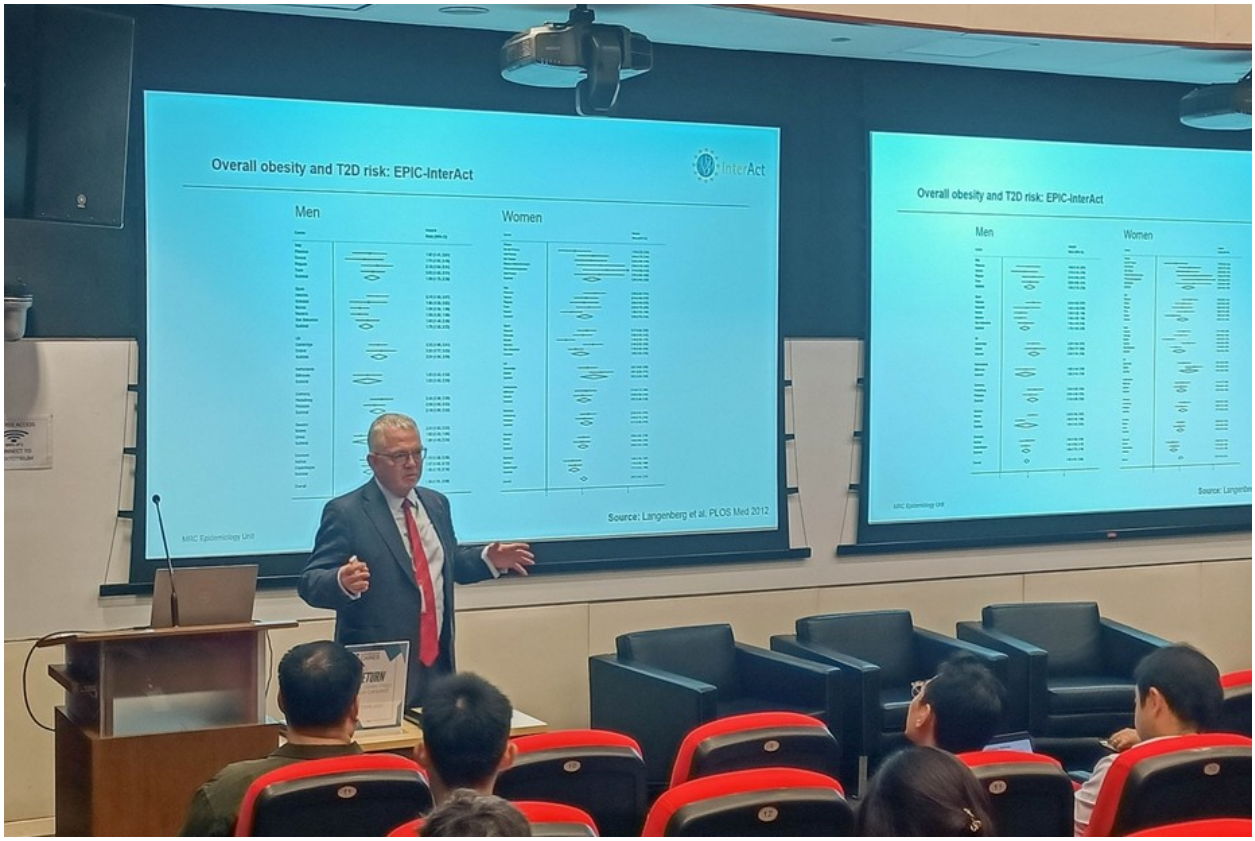
The **feasibility** will be demonstrated in terms of the ability to collect and process dynamic data characterising multiple features of the environment and the movement of people through the environment, and the ability to link geocoded environmental data with individual participant data from the SG100K study.

The **necessity** will be demonstrated in terms of showing the existence of relationships between environmental characteristics and health-related behaviours using the measures available in SG100K, and relationships between environmental characteristics, health-related behaviours, and clinical outcomes ascertained by linkage to electronic health record data.

In the future, Phase 2 will address the gaps in the **characterisation of the environment** identified in Phase 1 and will deploy at scale **dynamic approaches to the assessment of individual behaviour and environmental exposures** piloted in Phase 1. It will work in **close collaboration with SG100K** to determine how the characteristics of the environment and associations developed by the epidemiological analyses translate to **long-term population-level health outcomes**. It will **engage government agencies** in a bidirectional dialogue to support **active knowledge transfer**, identify **opportunities to study the impact of previous or current policy change** on the environment, behaviour and health in Singapore, and **co-create tools to inform future policy decisions** and **enhance the long-term impact of the programme**.

Scientific update

HD$_4$ started on 1st November 2024, with Cambridge investigators **Prof Nick WAREHAM (Programme Lead and PI, CAM)**, **Dr Ronita BARDHAN (Deputy Programme Lead and PI, CAM)** and researcher **Dr Jethro AKROYD (Scientific Programme Manager, CAM)** visiting CARES to launch the programme at the "Future of CARES Seminar" at the start of December 2024.



Prof Wareham gives a talk about strategies to improve public health at the "Future of CARES Seminar" on 6th December 2024.

The HD$_4$ team has since been busy recruiting. We recently welcomed existing CARES researchers **Ms Mei Qi LIM (Scientific Programme Manager, CARES)**, **Dr Kok Foong LEE (Software Developer, CARES), Ms Xinhong DENG (Sandra) (Software Developer, CARES)** and **Ms Yuan WANG (Research Associate, CARES)** to the programme and look forward to welcoming newly recruited researchers **Dr Jielin CHEN, Ms Ting ZHOU**, **Ms Sharyl CHIN** and **Dr Thi Ang Hong NGUYEN** in the coming weeks.

Cambridge team members **Prof James WOODCOCK (PI, CAM), Dr Thomas BURGOINE (PI, CAM),** and **Mr Oliver FRANCIS (Specialist Collaborator, CAM)** visited Singapore in February and March 2025 to support the recruitment process and to embed themselves at CARES.

The research team is now busy identifying key data sets, behavioural exposures and initial phenotypic endpoints in SG100K, and assessing the technical approach for handling the data. In the meantime, **Dr Ronita BARDHAN (Deputy Programme Lead and PI, CAM)** became the first investigator to publish work under the HD$_4$ banner with her paper, "*Harnessing street shade to mitigate heat stress: An in-situ parallel investigation under extreme heat conditions in tropical Singapore*" (DOI: 10.1016/j.scitotenv.2024.177864).

Previous studies have investigated the use of street shade with respect to outdoor thermal comfort, but the evidence base under extreme heat conditions is weak. This new study explores the cooling efficacy of diverse street shade types in mitigating urban heat in Singapore. We conducted in-situ measurements in a hot afternoon, measuring thermal and visual environments across 20 pairs of parallel sites (sunlit vs. shaded) in a high-density district. We analysed thermal comfort, represented by the Universal Thermal Comfort Index (UTCI), heat stress risks, and view factors of the sky, greenery, and buildings, and their interaction with heat stress relief. Our findings highlight three key points: Firstly, all street shade types improved outdoor thermal conditions, with average decreases of 0.8 °C in air temperature, 10 °C in mean radiant temperature, and 3.1 °C in UTCI. Secondly, street shade generally reduced heat stress severity by 20 % in the 'very strong heat stress' category and 12 % in the 'strong heat stress' category. Thirdly, the cooling efficacy of street shade was not solely dependent on changes in any single view factor. The results demonstrate the significant cooling benefits provided by street shade during extreme heat conditions. This study not only underscores the crucial role of street shade in mitigating heat stress but also offers valuable guidance to urban planners and designers in creating more liveable, sustainable, and climate-adaptive cities.

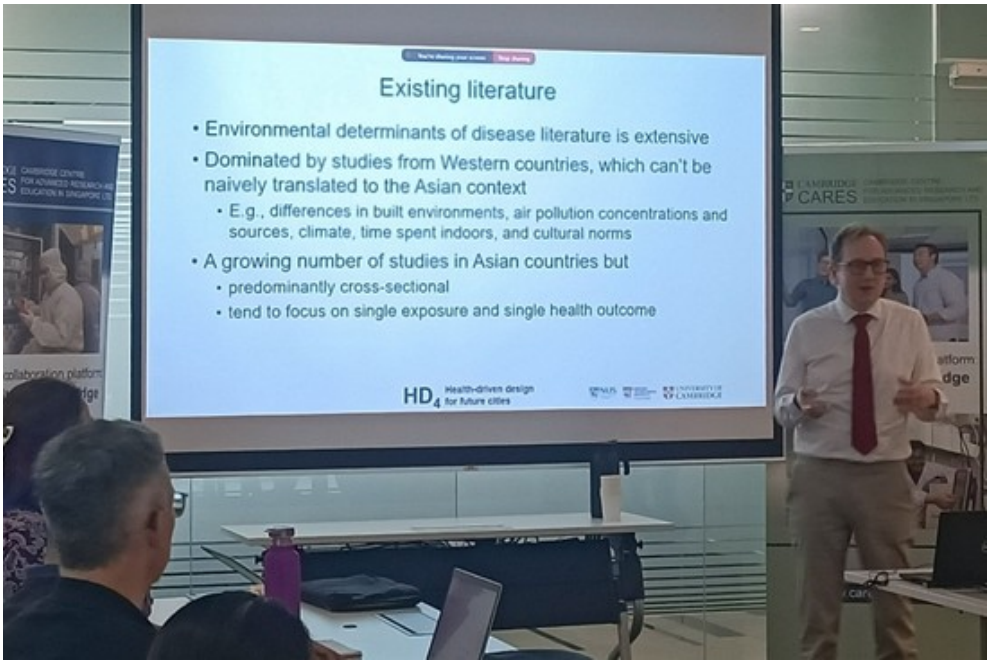
Prof Rudi STOUFFS (Deputy Programme Lead and PI, NUS) and researcher Ms Wang have had work relating to HD_4 accepted at international conferences. "*Impacts of Building Height and Local Climate Zones on the Performance of the InVEST Urban Cooling Model*" has been accepted as a full paper for oral presentation at the SBE25 Conference in Zurich, 25–27 June 2025. "*Revealing the Impact of 2D/3D Urban Morphology on Spatial Heterogeneity of Diurnal and Nocturnal UHI Through X-GeoAI Driven Analytics*" has been accepted for oral presentation at the 12th International Conference on Urban Climate (ICUC 12) in Rotterdam, 7 –11 July 2025.

Co-creation update

HD$_4$ has established the **Scientific Advisory Group (SAG)**, with confirmed representation from NEA, URA, NParks, MOHT, CLC, and S&TPPO colleagues. We are in active discussion with colleagues at HPB and HDB. The SAG forms a key component of our stakeholder engagement and co-creation strategy. They will be kept apprised of key developments and will provide strategic advice to the programme, supporting the development of inter-agency consensus and the translation of research outcomes that are implementable and contribute to the goals of the agencies.

Other activities and achievements

The team members visiting from Cambridge used the time at CARES to host a number of events. In February, CARES hosted a delegation from the Environment Agency in Abu Dhabi who learnt more about the opportunities presented by the HD$_4$ programme, which was presented by **Prof James WOODCOCK (PI, CAM)**. We hope that there may be an opportunity to develop a collaboration in the future. In March, Prof Woodcock hosted a seminar to showcase previous work and to socialise the HD$_4$ programme with other CREATE entities. At the end of the month, **Mr Oliver FRANCIS (Specialist Collaborator, CAM)** led a session focusing on how to communicate to achieve research impact, as part of a Communications Workshop for CARES researchers. The workshop also featured **Ms Olivia LEE (Communications Manager, CARES)** and Ms Jacqueline Garget from the University of Cambridge central communications team, who was visiting Singapore to help develop communications capacity at CARES.



Prof Woodcock presents to a delegation from the Environment Agency in Abu Dhabi who visited CREATE on 19th February 2025 to learn more about the HD$_4$ programme and city-related research from other CREATE entities.

Dr Thomas BURGOINE (PI, CAM) *introduces a seminar by Prof Woodcock to showcase previous work and socialise HD_4 at CREATE on 11th March 2025.*

Mr Francis leads a session with researchers from CARES at an Internal Communications Workshop on 20th March 2025.

AMPLE

AN ACCELERATED MANUFACTURING PLATFORM FOR ENGINEERED NANOMATERIALS

AMPLE is a direct result of C4T's research in sustainable reaction engineering. The project began in June 2022. The S$6.5M funded project seeks to translate annular flow microreactor technology to 100 kg/day scale production, utilising machine learning and an agile product development methodology. By pushing the technology to a TRL7/8 level, the team will overcome the scale-up "gap" for industrialisation of new material technologies.

Principal Investigator:

Professor Alexei LAPKIN
University of Cambridge

Project Lead:

Dr Nicholas JOSE
CARES

Since our last update, AMPLE has made significant strides towards a production ready technology. We have shifted our large-scale production system, the K100, to our partner manufacturing site in Malaysia (Elite Advanced Materials). Trials are ongoing to produce samples for end-users and potential clients, and provide a showcase for industrial partners. We have also successfully completed our seed round campaign, which has resulted in a significant investment into the company by lead investor UntroD, SGInnovate and Cambridge Enterprise Ventures. This funding will enable the company to scale its commercialisation of the K-series reaction systems to market. The team will continue operating in collaboration with CARES, working to develop next generation hardware and software to scale-up novel materials.

The reactor built in the CARES laboratory to scale up nanomaterials.

Other activities and achievements

AMPLE exhibited at Nanotech in Japan from 29–31 January 2025.

AMPLE has been engaging with industry in three key roles to establish a product-market fit: (1) suppliers (2) end-users and (3) distributors.

The following are the ongoing collaborations:

1. Suppliers: Vapourtec (UK)
2. End-users: Pfizer (USA), Asahi Kasei (JP), K+S (GER)
3. Distributors: Automed (IN), Kowa (SG/JP), Ehrfeld Microteknik (GER), Metlab (SG)

PIPS

PHARMA INNOVATION PROGRAMME SINGAPORE

PIPS is an industry-led platform coordinated by Singapore's Agency for Science, Technology and Research (A*STAR). PIPS aims to synergistically and strategically bring together public sector research capabilities and domain expertise of the pharmaceutical industry to enhance the productivity and operational efficiency within Singapore's pharmaceutical sector through leveraging novel manufacturing technologies and data analytics.

CARES is an academic partner in the PIPS programme and is leading two projects, one investigating the use of digital twins in pharmaceutical development and another focusing on data-driven solutions to rapidly identify environmental impacts in the chemical supply chain.

CARES Principal Investigators:

Professor Markus KRAFT
University of Cambridge

Professor Alexei LAPKIN
University of Cambridge

Automated Evaluation of Environmental Impacts of Pharma Manufacturing Processes

With funding from Pharma Innovation Programme Singapore (PIPS), via A*STAR

Automated Evaluation of Environmental Impacts of Pharma Manufacturing Processes is a three-year project that started in July 2023 funded by the Pharma Innovation Programme (PIPS 2) programme and led by **Prof Alexei LAPKIN (CAM)**. The project involves creating physical and machine learning based model libraries for upstream, downstream, wastewater treatment operations in pharma manufacturing processes, automatically assembling the models for a given target molecule, calibrating the models based on process needs, solving the models, and finally estimating the environmental impact of the process for a given production scale.

CARES has mostly sub-contracted the research and development work on this project to its spin-off company Chemical Data Intelligence (CDI) Pte Ltd. CDI has demonstrated the initial workflow of the complete solution. For the developmental work the company is using the case studies suggested by PIPS core member companies. In close collaboration with subject matter experts of the companies, CDI is developing the user environment for hosting the life cycle assessment prediction tool. In collaboration with the CARES team, the company is developing the individual modules for different components of the solution (reaction, separation, waste) and is starting to work on the integration of the modules.

Dr Dogancan KARAN (Senior Research Fellow, CARES) is in charge of the downstream and wastewater treatment libraries of the project.

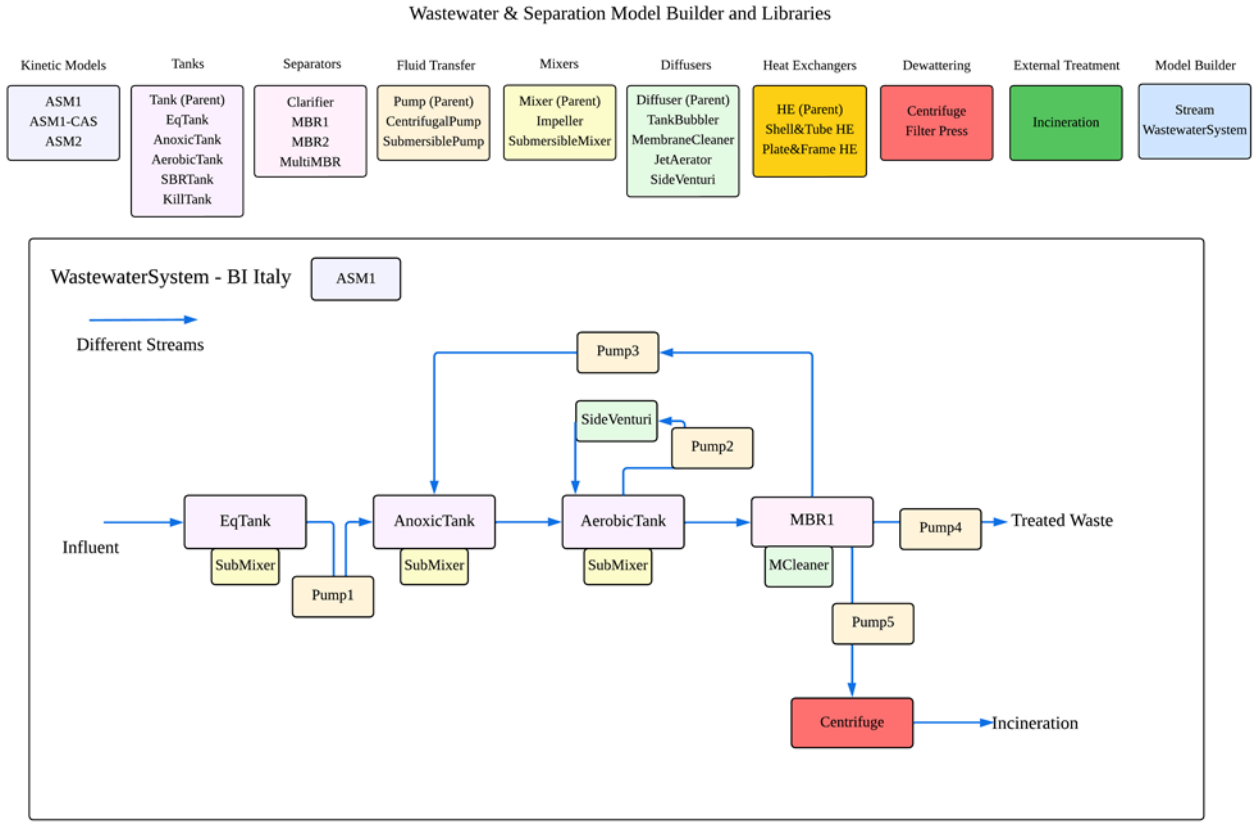


Figure 7.1: Schematic representation of the modelling environment created to simulate different wastewater processes. Different coloured boxes indicate a different class of unit operations.

Model libraries are created based on the industrial data gathered from different manufacturing sides of Boehringer Ingelheim. The industrial data involves wastewater freed properties, unit operation sensor readings, input/output streams, equipment information and properties of the hazardous waste treated off-site. This information is categorised to create a flexible plug-and-play style model building environment which consists of different unit operations calibrated against industrial data (Figure 7.1, top). This model environment can be used to create different processes to estimate their environmental impacts. An example of continuous activated sludge process (CAS) created by using the developed modelling environment is shown in Figure 7.1 (bottom). Dr Karan will be working on expanding the model library and simulating various processes to estimate their environmental impact.

From Digital Twins to Real Time AI-supported Plant Operation

With funding from Pharma Innovation Programme Singapore (PIPS), via A*STAR

This project is funded under the Pharma Innovation Programme Singapore (PIPS) programme and led by **Prof Alexei LAPKIN (CAM)**, **Prof Markus KRAFT (CAM)**, and **Dr Lianlian JIANG (A*STAR)**. This is a 2-year project that commenced in July 2023 and aims to demonstrate a methodology of management and development of physical models-based digital twins for pharmaceutical process development, operation, and management.

CARES' contribution to this project involves two main aspects: developing a generic formulation of physical models for processes (performed by the modelling team) and developing and/or extending existing process ontologies to instantiate ontology-based digital twins in the knowledge graph (performed by the ontology team). In this project, CARES also collaborates closely with the A*STAR Institute for Infocomm Research (I^2R), hereinafter referred to as the implementation team, to build and implement the digital infrastructure for the selected process. After numerous discussions and considering the project's ease of access, the Accelerated Manufacturing Platform for Engineered Nanomaterials (AMPLE) plant was selected to demonstrate the workflow developed within our project. (Read more about AMPLE on page 61).

During this reporting period, the modelling team completed the development of a knowledge graph framework for the digitalisation of chemical processes using models. The developed knowledge graph framework represents formulas and variables as interconnected nodes, associating them with relevant concepts applicable to both bottom-up and top-down chemical process modelling approaches. This knowledge graph infrastructure supports the implementation of various functional agents. For instance, agents encoded within the knowledge graph can interface with public chemical databases to supply essential physicochemical properties, thereby enhancing the modelling workflow.

The framework has been successfully demonstrated using a novel annular microreactor to characterise its mixing efficiency. Given formulas that describe kinetics and mixing mechanisms, the derived model has shown promise in accelerating reaction optimisation by effectively guiding experimental efforts. An amidation reaction was selected for validation. Pareto fronts were predicted under varying flow patterns using this knowledge graph framework and successfully contributed to identifying optimal operating conditions that balance space-time yield and *E*-factor. The ontology team also completed the develop-

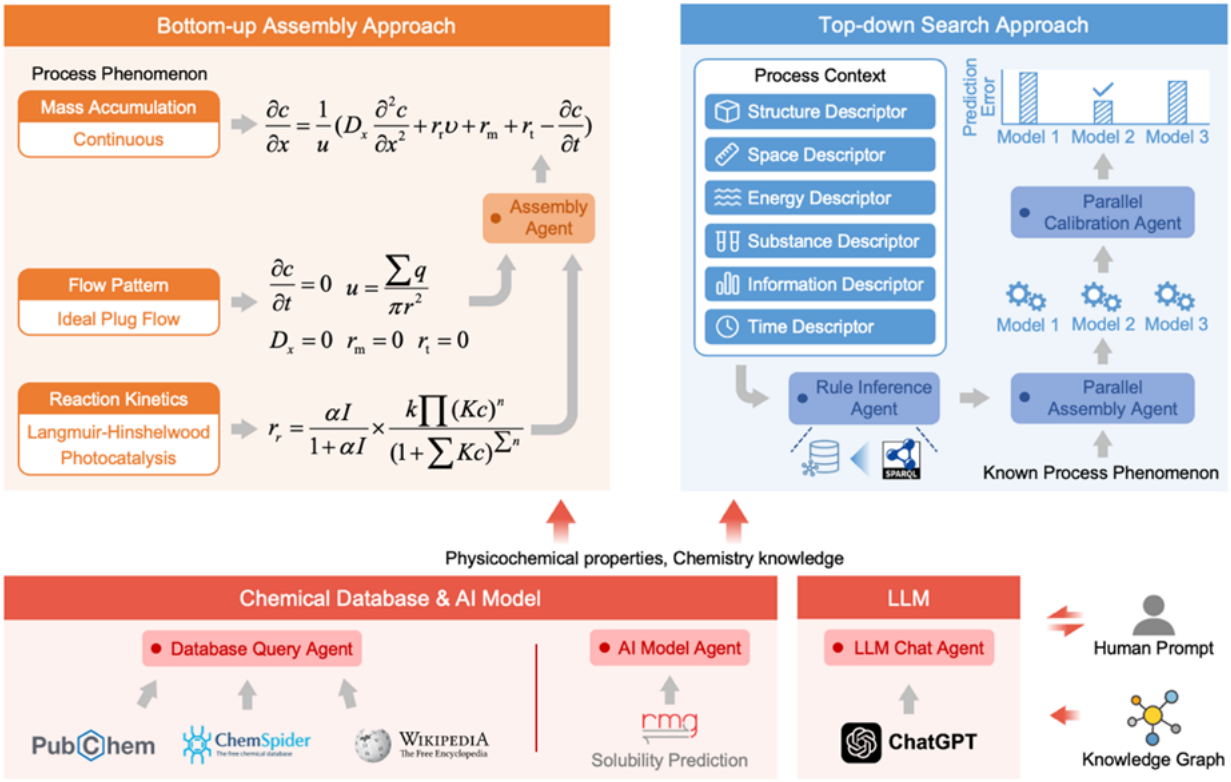


Figure 7.2: Schematic representation of the proposed knowledge graph framework for chemical process modelling.

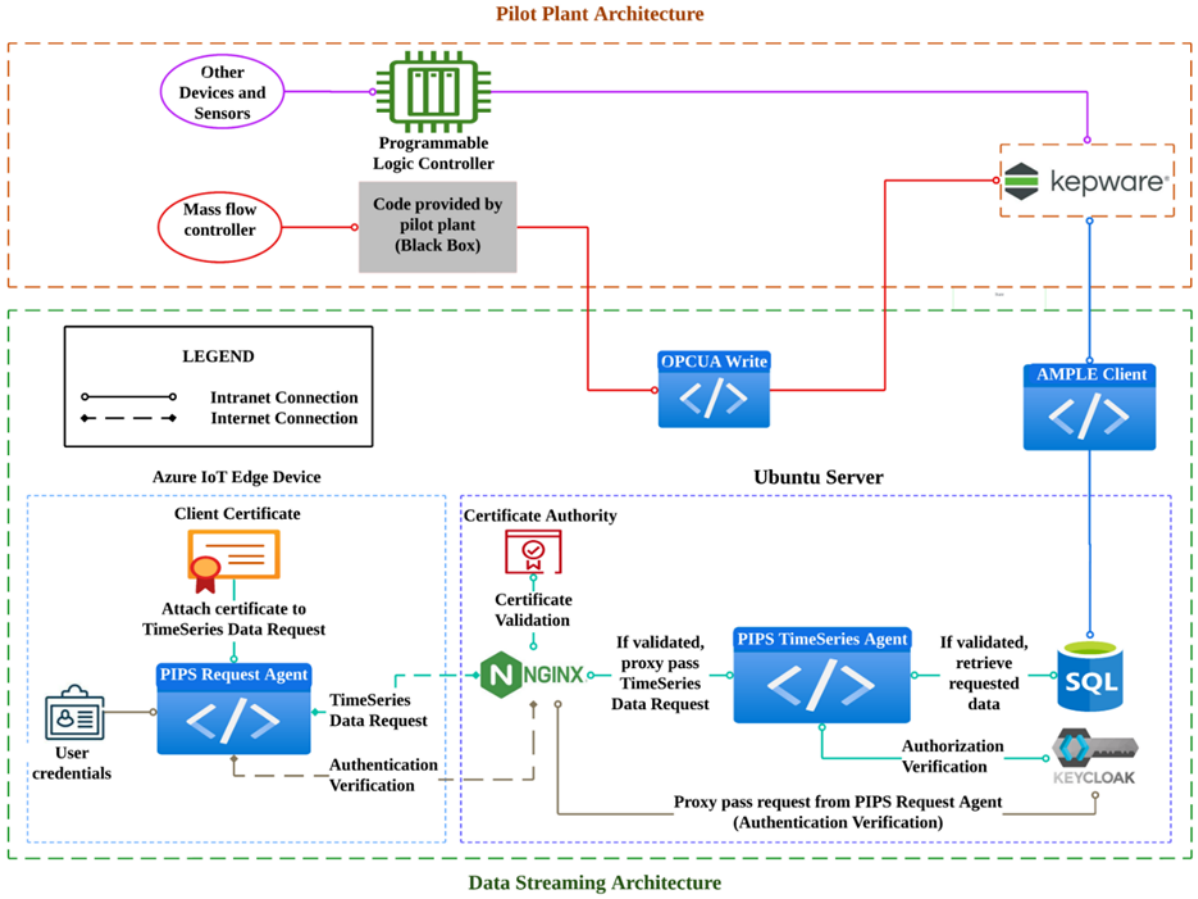


Figure 7.3: Data streaming architecture illustrating the data connectivity between the devices and sensors in the pilot plant, and the Azure IoT Edge Device.

ment of the data streaming architecture and associated software agents required to transmit data from the pilot plant's Kepware Open Platform Communications Unified Architecture (OPC-UA) server to an Azure Internet of Things (IoT) Edge Device, as illustrated in Figure 7.3. Data is being collected from various devices and sensors within the pilot plant and initially transmitted to the Kepware OPC-UA server. A series of software agents then parse, process, and securely transmit the data over a public internet connection to the Azure IoT Edge Device.

Two key security features have been implemented to ensure secure data handling: Keycloak is used for user authentication and authorisation, while Nginx is used for reverse proxying and client certificate validation.

Other activities and achievements

Dr Lianlian JIANG (PI, A*STAR), **Ms Srishti GANGULY (Assistant Project Manager, CARES), Dr Mohammed JERAAL (Materials Engineer, CARES),** and **Dr Yong Ren TAN (Research Fellow (Project Manager), CARES)** presented a poster and demonstration to explain the work done under the PIPS project at a GSK roadshow on 12th December 2024.

OTHER PROJECTS

OTHER CARES-FUNDED PROJECTS

In addition to C4T and CLIC, CARES hosts a number of other projects. These give our researchers an opportunity to explore new areas, develop technologies for commercialisation or build relationships with new industry partners or public sector collaborators.

The current CARES small projects include two projects in the Low-Carbon Energy Research (LCER) Phase 2 Programme, one hosted by NUS and one hosted by NTU.

These projects also provide a good opportunity for interns (such as Mr Hans GOH and Mr Seungjan CHA, pictured above) to have a novel experience of research and technology development not easily available during their undergraduate degrees.

Low-Carbon Energy Research Phase 2

In collaboration with the National University of Singapore

Dr B. HARIKRISHNAN (Research Fellow, CARES) has been actively contributing to the **LCER** project, which focuses on the development and application of the low order Incompletely Stirred Reactor Network (ISRN) for efficient parametric analysis of emissions at reduced computational cost. The ISRN serves as a post-processing tool that can utilise mixing fields generated from LES-CMC.

Numerical investigations were performed using the **LES-CMC** solver based on the experimental conditions of SINTEF sequential combustor operating with cracked ammonia fuel (Ditaranto and Saanum, 2024). A limited number of high-fidelity LES-CMC simulations serve as **anchor points** (Figure 8.1), from which detailed mixing field statistics are extracted and passed to the ISRN solver. The ISRN model is then employed to explore the design space of cracked-ammonia based gas turbines– such as pressure (P), fuel/air temperature (T), primary and secondary zone equivalence ratios (ϕ_{PZ} and ϕ_{SZ}), and ammonia decomposition ratio (DR).

Figure 8.2 (a) and (b) displays key mixing statistics (DR = 0.25 and $\phi_{PZ} = 1.5$), such as the time -averaged mixture fraction and its total variance (incorporating both resolved and sub-grid scale contributions). ISRN simulations have been extended to a range of DRs – 0.10, 0.20, 0.25, 0.6 and 0.9. Figure 8.2 (c) to (g) illustrates the temperature fields across these DRs, highlighting the interplay between the fuel composition and scalar dissipation rate, specifically near the burner. Figure 8.3 presents the emission distribution along the axial direction, providing insights into pollutant formation trends.

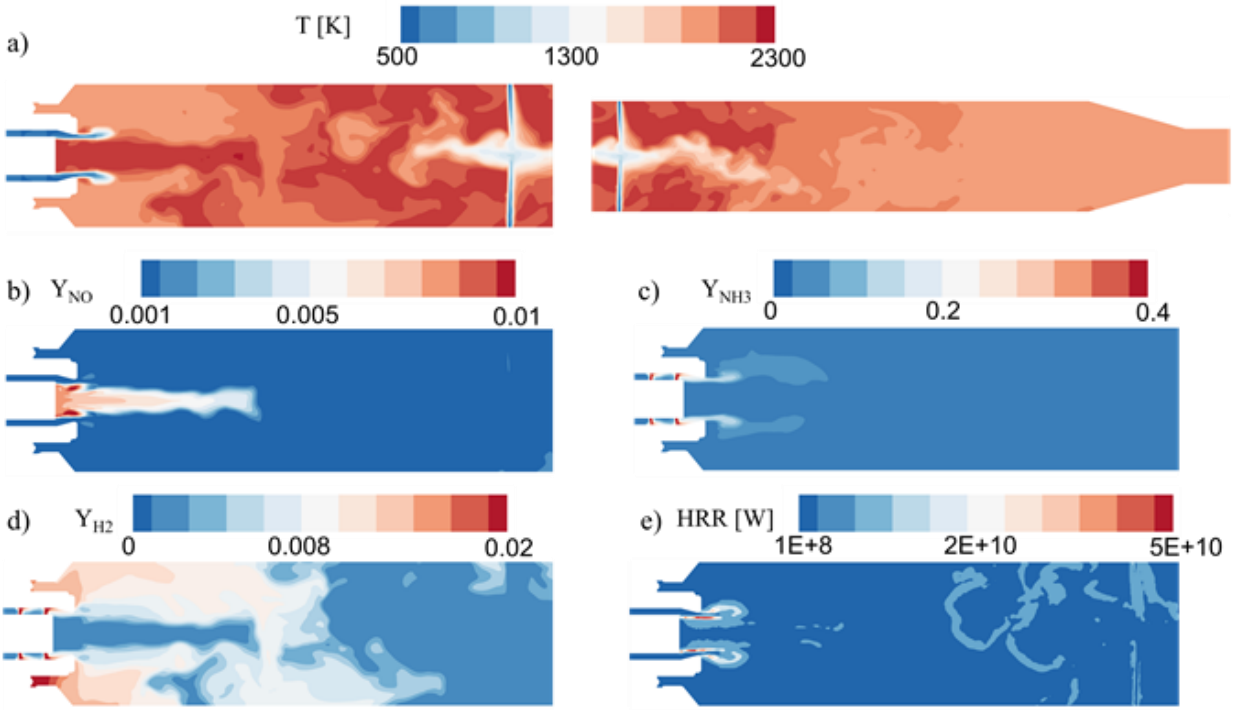


Figure 8.1: LES-CMC results for DR = 0.25 and $\phi_{PZ} = 1.5$. a) Temperature, b) mass fraction of NO, c) mass fraction of NH_3, d) mass fraction of H_2 and e) heat release rate.

Dr B HARIKRISHNAN

To further assess the predictive capability of ISRN, additional LES anchor simulations are planned. These will support a more comprehensive design-space exploration via ISRN. A subset of LES runs will also be used to validate ISRN predictions.

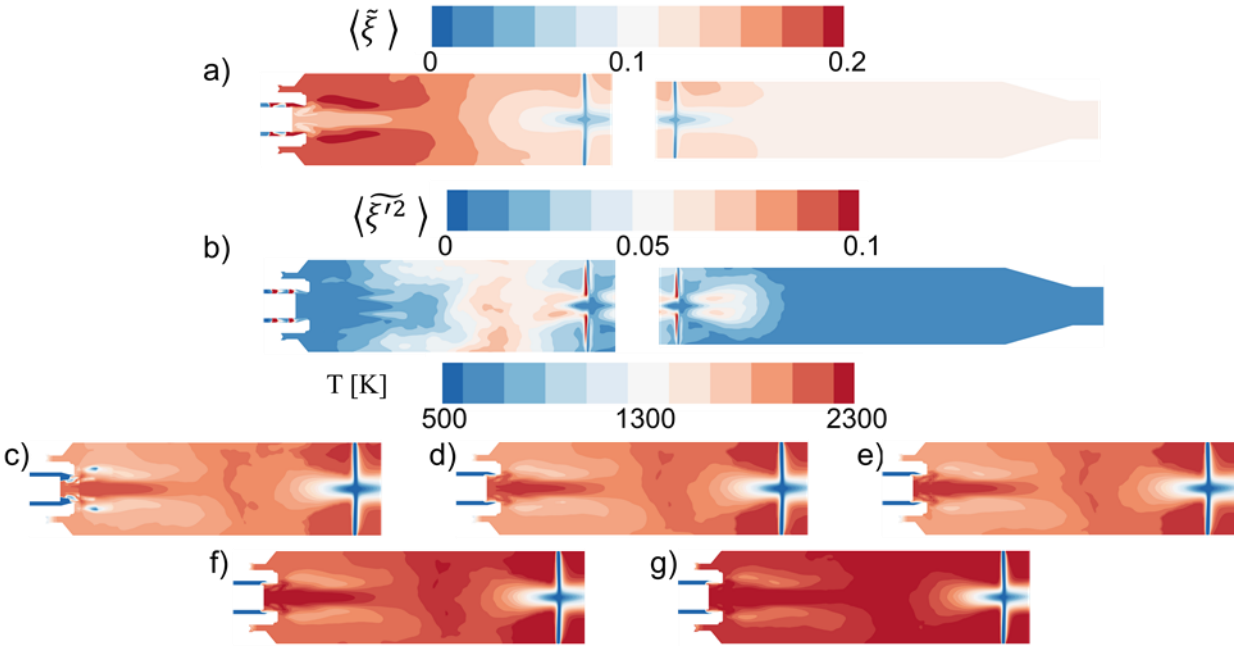


Figure 8.2: Mixing field data from LES of case with decomposition ratio 0.25 and $\phi_{PZ} = 1.5$ *- (a) Time-averaged mixture fraction, (b) its total time variance. Corresponding ISRN simulations for decomposition ratios of (c) 0.10, (d) 0.20, (e) 0.25, (f) 0.60 and (g) 0.90.*

Dr B HARIKRISHNAN

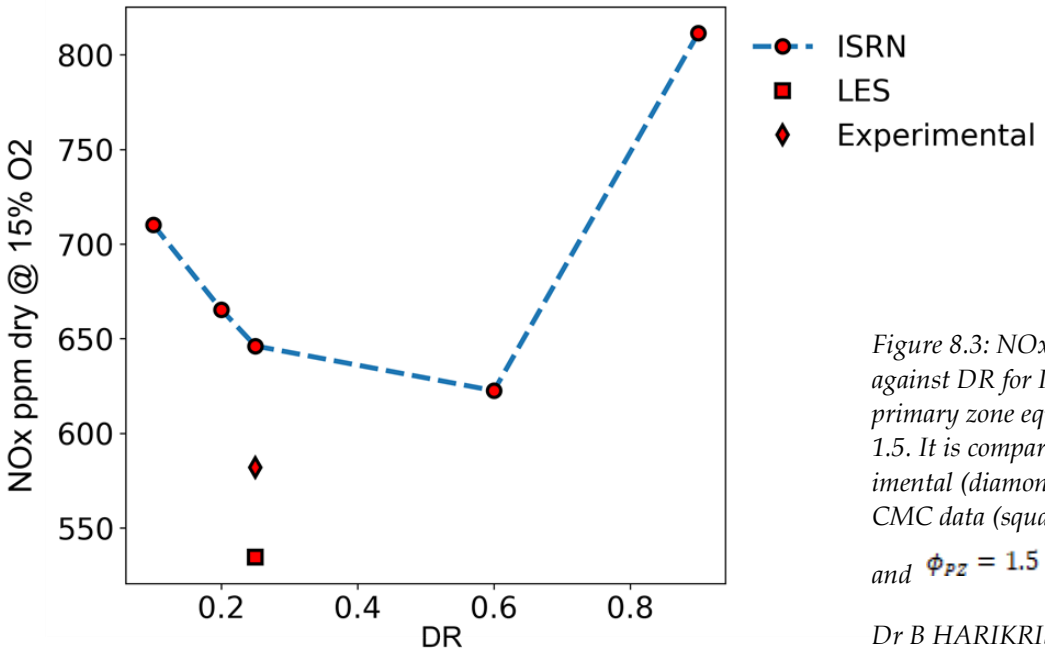


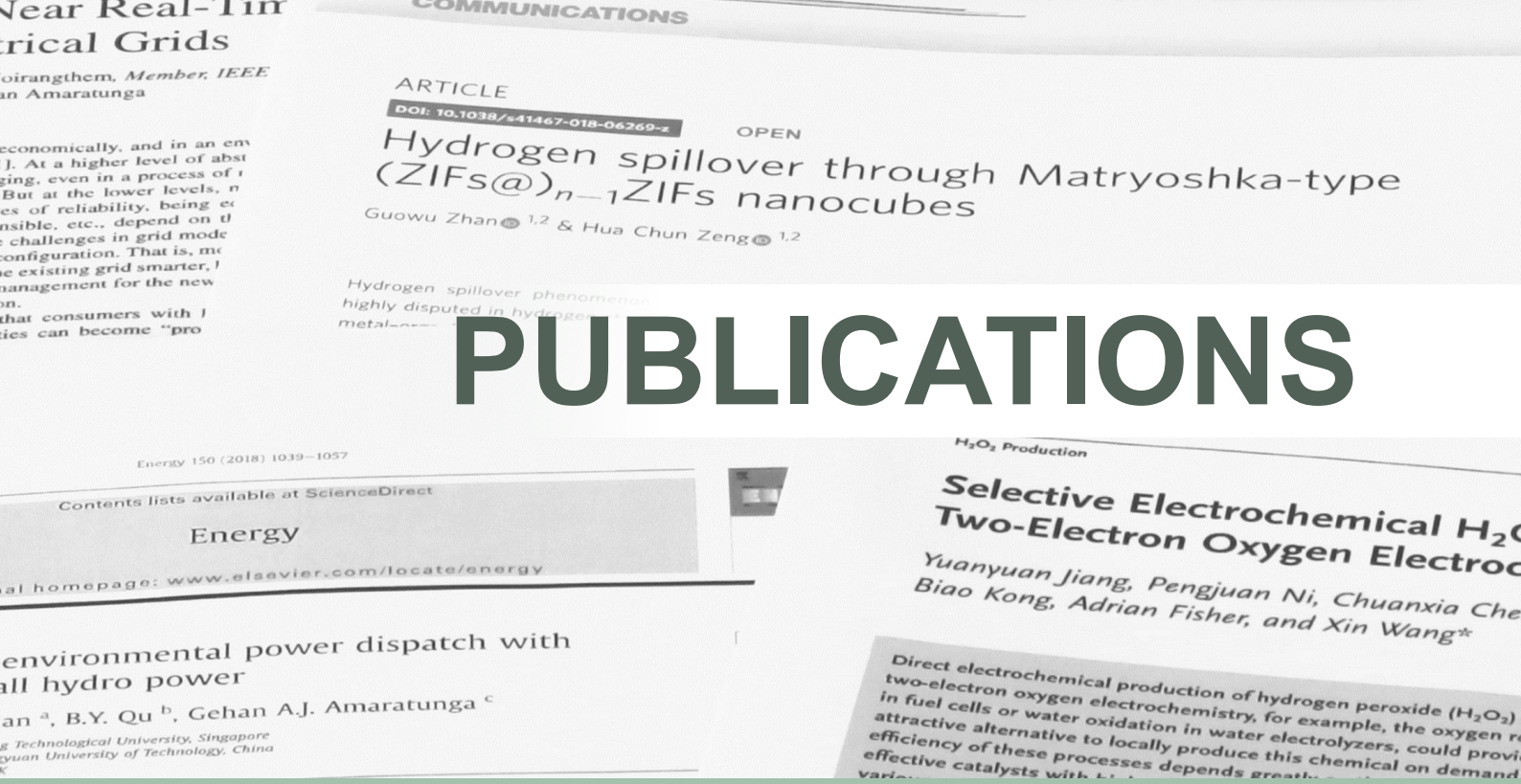
Figure 8.3: NOx emissions against DR for ISRN cases for primary zone equivalence ratio 1.5. It is compared against experimental (diamond) and LES-CMC data (square) at DR = 0.25 and $\phi_{PZ} = 1.5$ *.*

Dr B HARIKRISHNAN

Other activities and achievements

Dr B. HARIKRISHNAN (Research Fellow, CARES) has two papers accepted for upcoming conferences:

- B. Harikrishnan, S. Gkantonas and E. Mastorakos (2025). Large Eddy Simulation of Dual-Fuel Swirl Flames. 13th Mediterranean Combustion Symposium in Corfu, Greece from 1–5 June 2025.
- Harikrishnan and E. Mastorakos (2025). Predictive modelling of ammonia combustion systems: Coupled LES-CMC and ISRN approach. 11th International Symposium on Turbulence, Heat and Mass Transfer in Tokyo, Japan from 21–25 July 2025.



PUBLICATIONS

ALL PUBLICATIONS WITH CREATE ACKNOWLEDGEMENT

The following list includes all the C4T publications from the period of the C4T impact-focused "CN" projects starting November 2023. Those in bold are new for this reporting period. For a full record of Phase 1 and Phase 2 publications (April 2013—October 2023) please visit our Publications page on the CARES website: www.cares.cam.ac.uk/publications/

C4T impact-focused "CN" projects

- Bai, Jiaru, Kok Foong Lee, Markus Hofmeister, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft. 2024. 'A Derived Information Framework for a Dynamic Knowledge Graph and Its Application to Smart Cities'. *Future Generation Computer Systems* 152 (March):112–26. https://doi.org/10.1016/j.future.2023.10.008.
- Bai, Jiaru, Sebastian Mosbach, Connor J. Taylor, Dogancan Karan, Kok Foong Lee, Simon D. Rihm, Jethro Akroyd, Alexei A. Lapkin, and Markus Kraft. 2024. 'A Dynamic Knowledge Graph Approach to Distributed Self-Driving Laboratories'. *Nature Communications* 15 (1): 462. https://doi.org/10.1038/s41467-023-44599-9.
- **Chang, Jinquan, Sikai Wang, Max J. Hülsey, Sheng Zhang, Shi Nee Lou, Xinbin Ma, and Ning Yan. 'Electrothermal Conversion of Methane to Methanol at Room Temperature with Phosphotungstic Acid'. *Angewandte Chemie International Edition* 64, no. 5 (27 January 2025): e202417251. https://doi.org/10.1002/anie.202417251.**
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