CAMBRIDGE CARES

www.cares.cam.ac.uk

A research collaboration platform: University of Cambridge and Singapore

Biannual Research Report April - September 2025

COVER IMAGE

Dr Raudah Lazim (right) presenting to Mr Tharman Shanmugaratnam (President of the Republic of Singapore) (third from the left) with Prof Deborah Prentice (Vice-Chancellor of the University of Cambridge) (second from right) listening in.

Photo credits: Cambridge CARES/Back Button Media

PRODUCED BY

CAMBRIDGE CENTRE FOR ADVANCED RESEARCH AND EDUCATION IN SINGAPORE LTD.

Registration No. 201302109Z

1 Create Way, #05-05 CREATE Tower

Singapore, 138602

enquiries@cares.cam.ac.uk

www.cares.cam.ac.uk

Content Page

Foreword 2

About Us 4

Programme Updates

C4T 6

CLIC 19

HYCOMBS 26

SM_3 33

HD_4 38

AMPLE 46

PIPS 48

OTHER PROJECTS 51

Publications 54

Foreword

The biannual preparation of this report brings to mind the first version created after the launch of the Cambridge Centre for Carbon Reduction in Chemical Technologies (C4T) programme in 2013.

As C4T draws to a close with a last update in this report, we give thanks to the National Research Foundation in Singapore for investing the time and resources into C4T which has shown tremendous impact and contribution to fundamental research (730+ papers and an H-index of 106 to date), technology development (34 invention disclosures, 20 patent filings and 4 licenses), and translational impact (6 spin-off companies).

We must also acknowledge the numerous Principal Investigators, Co-Investigators, Research Fellows, PhD students, research staff, graduate trainees, and the corporate team who have kept C4T vibrant. As Cambridge's first overseas research centre, we are inspired to continue our journey in Singapore with strength and purpose, mirroring Cambridge's long-lasting commitment to solve global challenges. It is with delight that we have new projects to continue sharing (HYCOMBS, SM_3, HD_4) with the public.

President of the Republic of Singapore visit July 2025

President Tharman Shanmugaratnam visited the CARES lab in July 2025 as part of a larger visit hosted by the National Research Foundation to hear updates from the CREATE Thematic Programme in Decarbonisation. We presented the two CARES-hosted projects: hydrogen and ammonia combustion (HYCOMBS) and chemical network analysis (SM_3). The project leads spoke with President Tharman to explain their reasons for conducting the research in Singapore, and we highlighted our Research Fellows as local talents in their field. The visit provided a fantastic spotlight for CARES as a hub for decarbonisation.

CLIC outreach in Cambridge

Our lifelong learning research programme, CLIC, brings their research to the Cambridge public in September 2025 with parallel workshops targeting different age groups and an evening reception reflecting on the nature of policy and research. The latter event included an invited guest from the Ministry of Education in Singapore who shared his insight working with research centres, and specifically CLIC, to ensure that policy continues to be forward-thinking and long-term. While CLIC's research focuses on the Singaporean population, we were delighted with the enthusiasm from our UK audience for understanding the importance of learning and creativity in their own lives.

HD4 stakeholder engagements

The Health-driven design for cities (HD_4) programme understands that to investigate the effect of Singapore's urban environment on residents' health outcomes and behaviours, they must first understand Singaporeans.

HD_4 has taken huge strides in setting up and completing a successful first Stakeholder Advisory Group meeting. The intention is to meet regularly with representatives from Singapore agencies, who will ensure the close connectivity with local knowledge by advising on changes and informing the research direction. The team also hosted a Summer Seminar Series, drawing over 120 attendees to a series of lectures from visiting Cambridge Professors over the months of July and August.

We hope you have enjoyed reading the highlights from CARES in the last 6 months. 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.

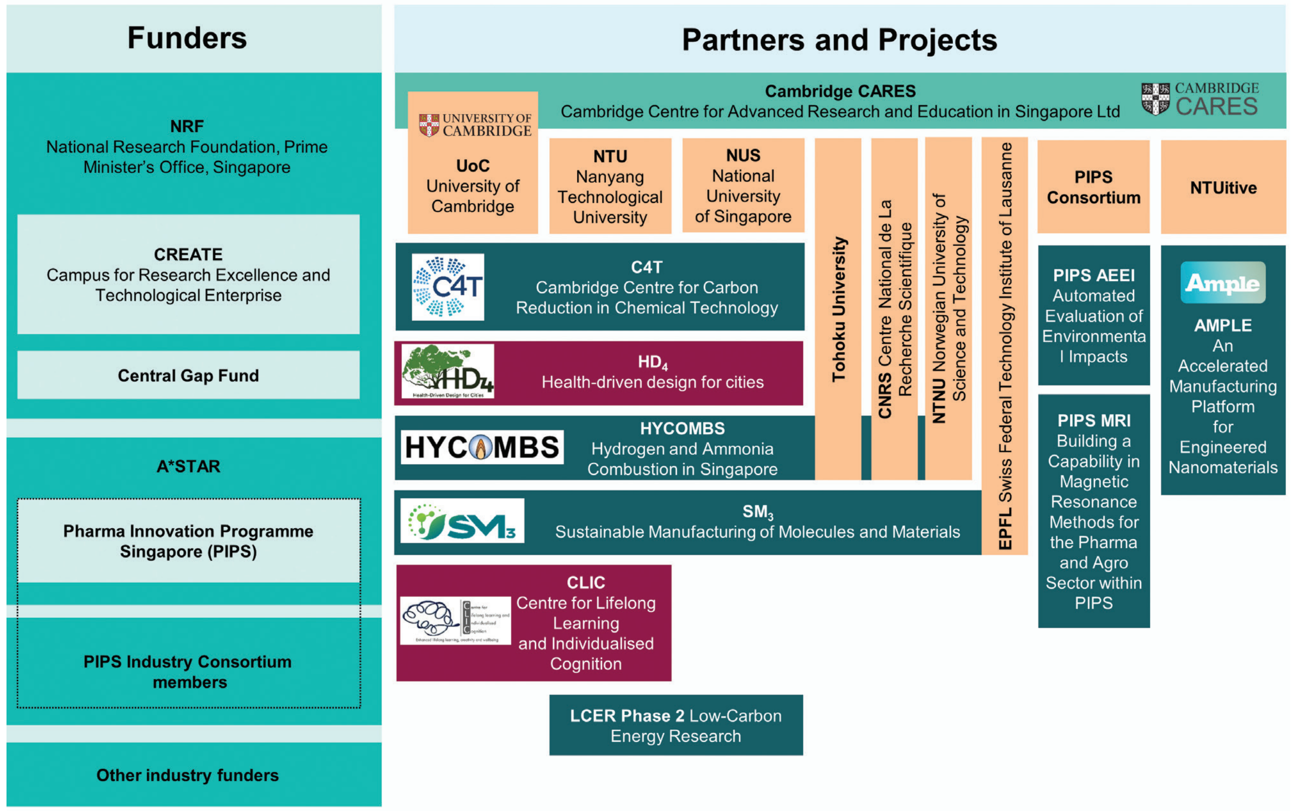
The first programme administered by CARES, the Cambridge Centre for Carbon Reduction in Chemical Technologies (C4T), is entering its final phase after 12 years. The motivation for C4T was to provide a rich pipeline of scientific insight and technological innovation with high potential for positive results within the decarbonisation agenda if deployed by appropriate industry and government parties.

The C4T programme is a world-leading partnership between Cambridge and Singapore, with the first five-year research phase focused on assessing and reducing the carbon footprint of the integrated petro-chemical plants on Singapore's Jurong Island.

The programme received a further five years of funding for Phase 2, which commenced in November 2018 and will complete in October 2025. This next phase considered that decarboisation must be addressed at all levels — from fundamental science to the development of low-carbon alternatives of key technologies, to identifying deployment opportunities, and exploiting synergies across research groups.

C4T's impact and contribution to fundamental research (730+ papers and an H-index of 106 to date), technology development (34 invention disclosures, 20 patent filings and 4 licenses), and translational impact (6 spin-off companies), is evident. The programme has also hosted 47 PhD students, some with matched industry funding through the Cambridge-CARES studentship scheme. As C4T draws to a close, we celebrate the programme's legacy and platform for kickstarting our new decarbonisation projects.

In July 2024, NRF announced a new SGD$90m Decarbonisation programme. The two CARES-hosted projects under this initiative 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. Additionally, a Cambridge Professor is also a partner on two other projects: eCO_2RR hosted by NUS and NH3-SOFC hosted by NTU and Imperial College London.



AMPLE (An Accelerated Manufacturing Platform for Engineered Nanomaterials), funded by the Central Gap Fund, is also in its final phase at CARES. AMPLE grew from research within the C4T programme and is bringing products to commercialisation via the spin-off company, Accelerated Materials, which recently completed their seed round campaign in April 2025.

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

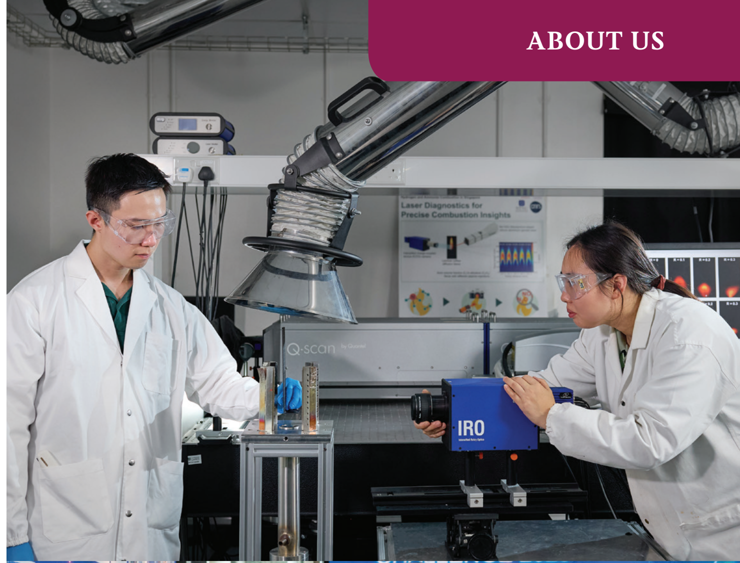
The Health-driven design for cities (HD_4) programme commenced in October 2024, contributing to CARES' portfolio on human health and potential. HD_4 will use data from the SG100K study to investigate the relationships of the built environment on the behaviour and health outcomes of Singaporean residents.

There are currently two ongoing streams under the Pharmaceutical Innovation Programme Singapore (PIPS); one stream focuses on using data-driven solutions to rapidly identify environmental impacts in the chemical supply chain, the other stream will use magnetic resonance imaging to optimise operating conditions for heterogeneous hydrogenation reactions in continuous-flow microscale trickle-bed catalytic reactors.

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 on our website.

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



Project Leads

Professor Markus KRAFT
University of Cambridge

Professor Rong XU
Nanyang Technological University

Professor Ning YAN
National University of Singapore

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.

SUSTAINABLE REACTION ENGINEERING

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

Principal Investigators

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 methanation using Ni/alkaline earth metal carbonate dual-function materials (DFMs). She was investigating kinetic reaction model on the hydrogenation of the Ni-amorphous $CaCO_3$ based. She discovered that different solid-state reaction models governing the hydrogenation kinetics on the Ni/$CaCO_3$ DFMs during the fast- and slow-stage hydrogenation (Figure 1.1). The simulated model expression fits the experimental data well (Figure 1.2). She is now preparing a manuscript of this work for future submission and publication.

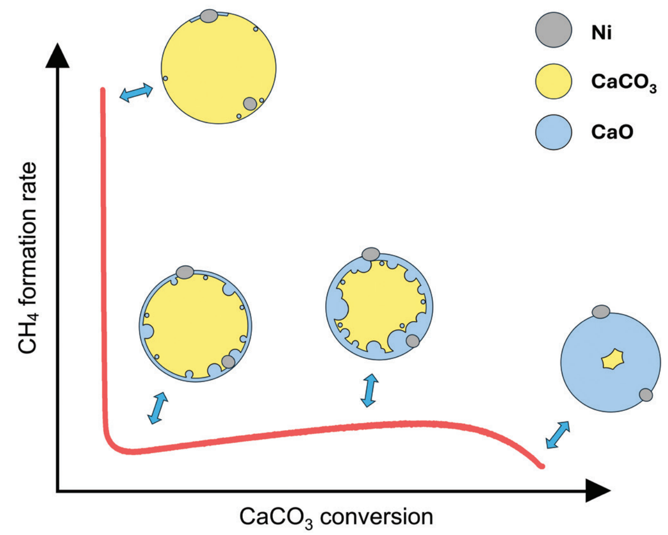


Figure 1.1: Schematic mechanism of the overall reaction model for the hydrogenation of Ni/$CaCO_3$ during the ICCU cycles at 400 °C.

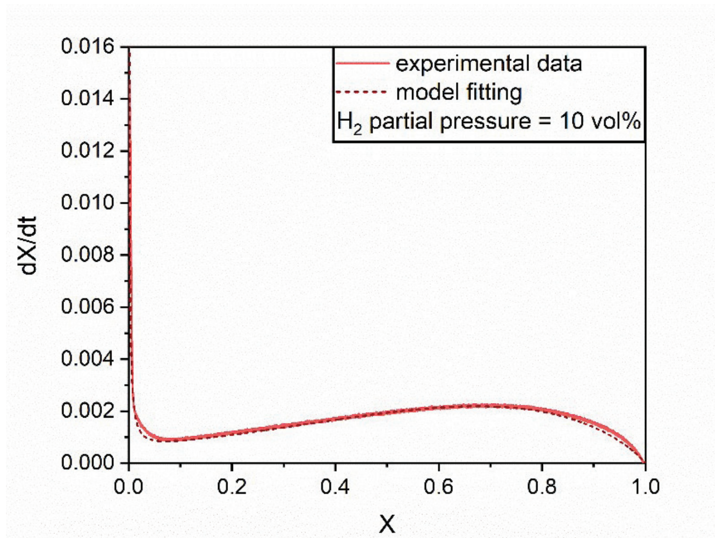


Figure 1.2: Overall reaction model fitting for the hydrogenation of Ni/$CaCO_3$ DFMs during the ICCU-Methanation cycles, in 10 vol% H_2/N_2 at 400 °C.

ELECTROCHEMISTRY

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

Principal Investigators

Prof Adrian FISHER (CAM)

Prof Zhichuan XU (Jason) (NTU)

Assoc Prof Sui ZHANG (NUS)

Dr Qikai SHEN (Research Fellow, NTU) has designed a bifunctional ammonia-oxidation catalyst spatially decoupling NH_3 activation and *OH adsorption to overcome the intrinsic trade-off of single-component systems. Atomically dispersed Zn single atoms in an N,O-doped carbon support (Zn_1/NOC) serve as dedicated *OH-adsorption sites, while Ir-modulated Pt(100) nanocubes selectively activate NH_3. Comprehensive structural characterisation (AC HAADF-STEM, XPS, XANES, EXAFS) confirms $Zn\text{-}N_3O_3$ coordination and atomically isolated Zn centers. Electrochemical-kinetic analysis, mechanistic spectroscopy, and DFT calculations reveal that Zn_1/NOC lowers the *OH-adsorption energy by 0.84 eV (to −0.98 eV versus −0.14 eV on Pt), facilitating the dehydrogenation steps and reducing surface poisoning. Simultaneously, traces of stabilised Ir^{4+}-decorated Pt cubes enhance NH_3 dissociation kinetics to form N_2. The catalyst demonstrates a specific activity of 3.80 mA cm^{-2}_{PGMs}, exceeding the state-of-the-art benchmarks. When deployed in a membrane-electrode-assembly direct ammonia fuel cell, the catalyst achieves a maximum current density of 200 mA cm^{-2} and a peak power density of 18 mW cm^{-2}, representing a significant improvement over previously reported systems, with ~250% increase over Pt_{np}–C || Pt/C and more than double monofunctional systems. This work demonstrates a generalisable strategy for engineering spatially decoupled active sites in multistep electrochemical reactions, paving the way for high-performance ammonia fuel cells and beyond.

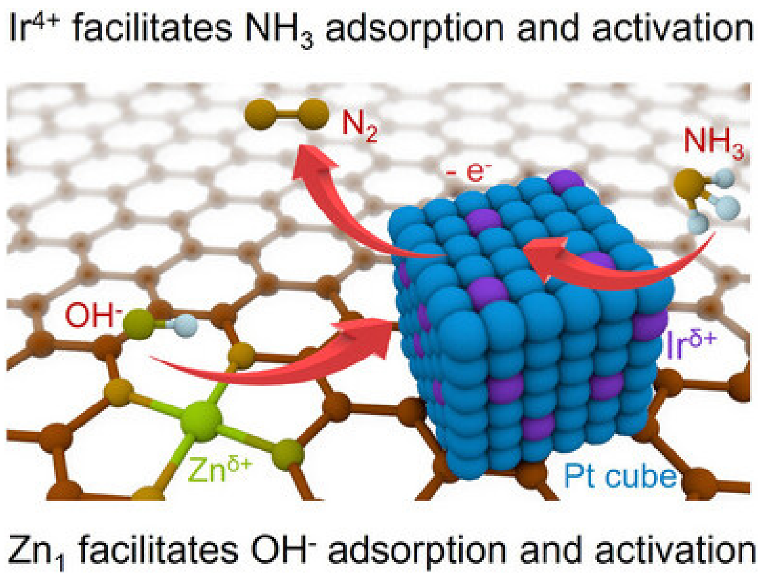


*Figure 2.1: Monodisperse $Zn_1N_3O_3$ and Ir^{4+} synergistically modulate substrate and active sites for high-performance ammonia oxidation. Atomically dispersed Zn single atoms in an N,O-doped carbon support serve as dedicated *OH-adsorption sites, while Ir-modulated Pt(100) nanocubes selectively activate NH_3.*

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

Principal Investigators

Prof Adrian FISHER (CAM)

Prof Zhichuan XU (Jason) (NTU)

Dr Chencheng DAI (Research Fellow, NTU) has employed a proton exchange membrane (PEM) electrolyser to improve the glycerol electrolysis activity, selectivity towards higher value products, and reduce production cost. The most valuable GOR products are dihydroxyacetone (DHA) and glyceraldehyde (GLAD); however, they are not stable and decompose in an alkaline environment. Nevertheless, the lack of hydroxide ion supply in neutral and acidic electrolytes can sacrifice the GOR activity and therefore increase production cost. To overcome these limitations, a PEM electrolyser can be used to promote the GOR activity by enhanced mass transfer and reduced resistance. Meanwhile, the MEA structure allows the usage of glycerol/water solution directly without additional supporting electrolyte (e.g. KOH), which can greatly reduce the production cost. To achieve an industrial-level current density of 0.2 A cm^{-2}, the cell voltage of only 0.57 V (chronoamperometry (CA)) is required, and the molar selectivity towards GLAD & DHA of 46% can be achieved. Meanwhile, the pulse voltametry (PV) can further increase the molar selectivity to 55% at an industrial-level current density of 0.2 A cm^{-2}.

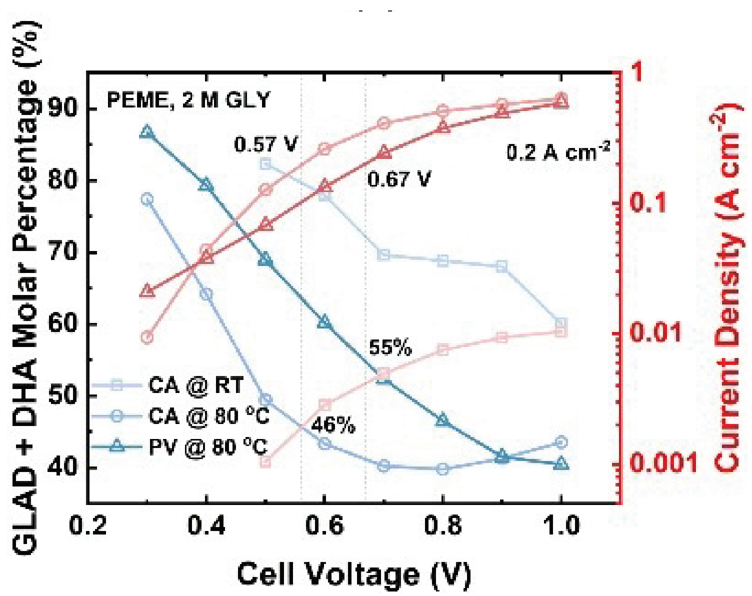


Figure 2.2: The comparison of molar percentage towards GLAD and DHA production and average current density of glycerol electrolysis in PEME via CA and PV methods at RT and 80 °C.

MARITIME DECARBONISATION

CN9: Dispersion modelling and air quality changes by switching to new marine fuels

Principal Investigators

Prof Epaminondas MASTORAKOS (CAM)
Prof Markus KRAFT (CAM)

Dr Li Chin LAW (Research Fellow, CARES) has recently completed the first phase of research work in collaboration with **Laskaridis Shipping Co. Ltd. and METIS Cyberspace Technology**. The two years of historical data (2023 and 2024) were analysed using a newly developed **in-house Voyage Analyser tool by EMICAST Pte. Ltd.** EMICAST is a spin-off founded by Dr Law. The research is structured into two parts. Part I focuses on developing a data-driven conceptual design framework that utilises historical ship operational data to design various low-emission integrated systems for a reference bulk carrier. For example, a post-combustion carbon capture system (CCS) was designed and hydraulically verified in Aspen HYSYS to operate effectively across 30–100% engine load conditions. The pre-combustion CCS configuration was optimised to maximise the carbon reduction rate, while alternative fuel systems were designed with optimal containment sizing to meet voyage energy requirements without conventional oversizing. Part II builds on these conceptual designs to evaluate the techno-economic performance of various low-carbon pathways under different regulatory scenarios (conservative, moderate, optimistic), using integrated cost and CO_2 avoidance metrics. These assessments account for revenue losses due to reduced cargo capacity, regulatory penalties and incentives, fuel-related operating cost (OPEX), and system capital investment (CAPEX). An important finding of the work is that incentivising over-compliant vessels is critical to accelerate the adoption of such solutions. Future work will extend the analysis to different vessel types and sizes, each operating under varied voyage profiles, to examine how these parameters influence the performance of low-carbon technologies.

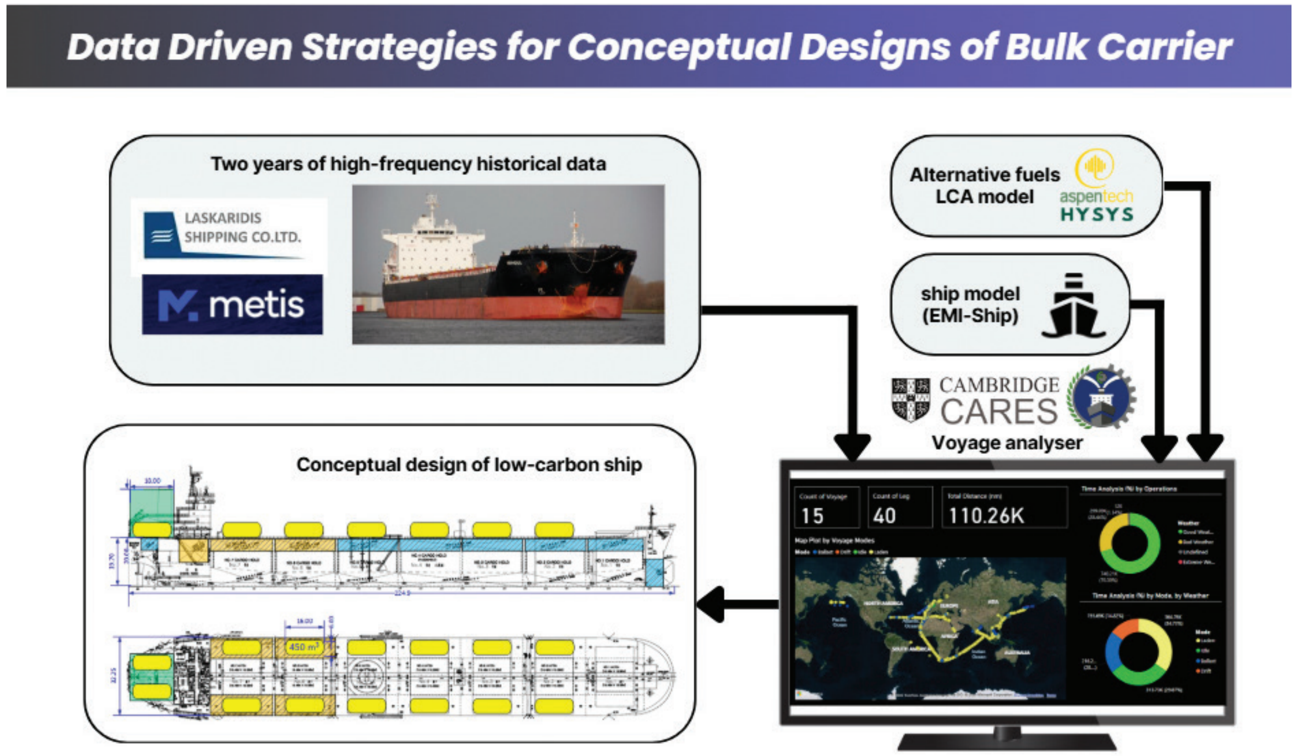


Figure 3.1: The voyage analyser invented in this study is capable of transforming historical ship data into important insights such as voyage pattern and operational profile. Additionally, LCA modelling, and ship performance modelling are integrated to generate operational and fuel consumption profiles for conceptual design and quantitative assessment of selected low-carbon alternatives.

CN14: Alternative marine fuel engine modelling

Principal Investigators

Prof Epaminondas MASTORAKOS (CAM)

Dr B. HARIKRISHNAN (Research Fellow, CARES) contributed to the development of the in-house solver **dcmcConverge**, tailored for investigating dual-fuel spray combustion using large eddy simulation (LES). The solver was applied to study the UCAM bluff-body stabilised dual-fuel swirl flame experiment, which involves n-heptane injected into a premixed methane/air stream entering the combustor through an annular passage after passing a swirler. This configuration serves as a representative model for staged combustion systems and fuel-flexible gas turbines operating under varying fuel compositions.

Two operating conditions were examined, below and above the lower flammability limit (LFL), with values of $\phi_{premixed}$ = 0.14 and $\phi_{premixed}$ = 0.56, respectively.

The simulations revealed a clear transition in flame structure: at the lower ratio, combustion exhibited spray-dominated, diffusion-controlled behaviour, while at the higher ratio, the flame displayed features of a premixed flame, aligning with experimental observations (Sidey and Mastorakos, 2018).

Further analysis was conducted in both the physical space and passive scalar space, providing deeper insight into the flame's stabilisation and mixing characteristics. These analyses helped elucidate the coupling between fuel evaporation, turbulent mixing, and chemical reaction processes that govern dual-fuel behaviour.

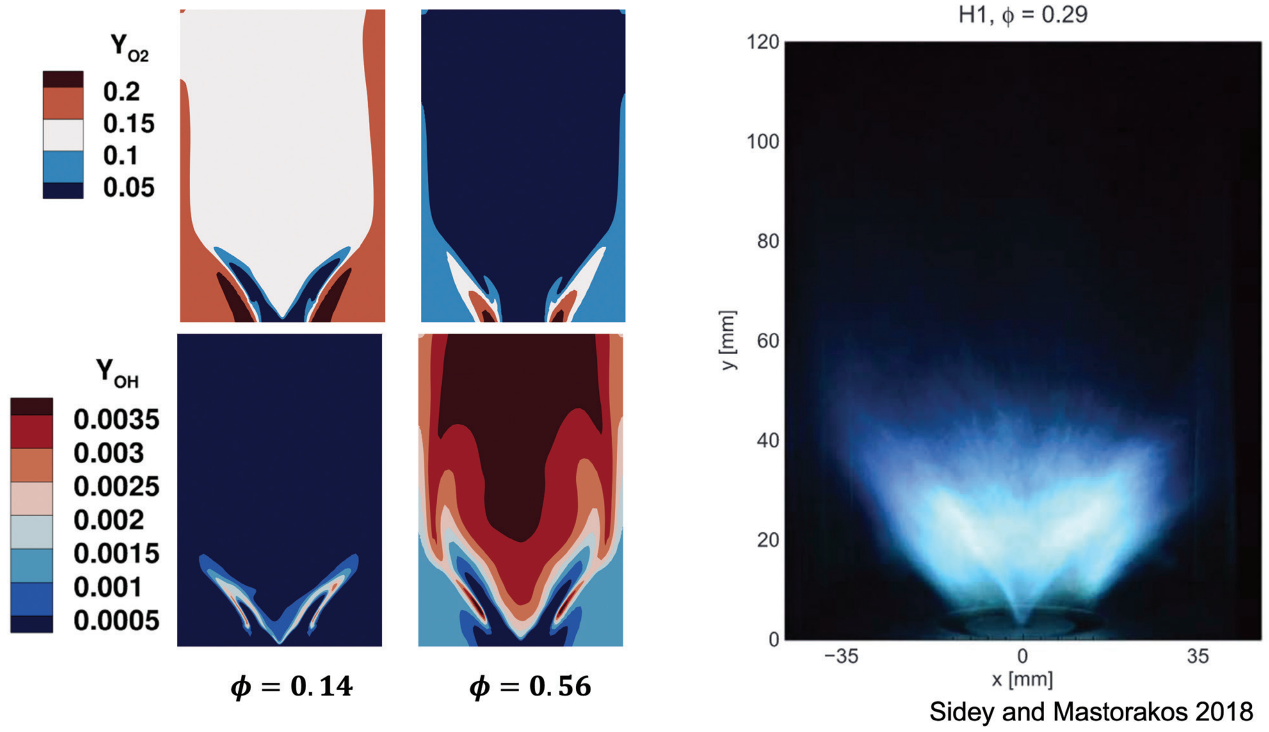


Figure 3.2: Comparison of species mass fractions for premixed equivalence ratio ($\phi_{premixed}$) of 0.14 and 0.56. Comparison is shown with the pure n-heptane flame by experiments of Sidey and Mastorakos 2018.

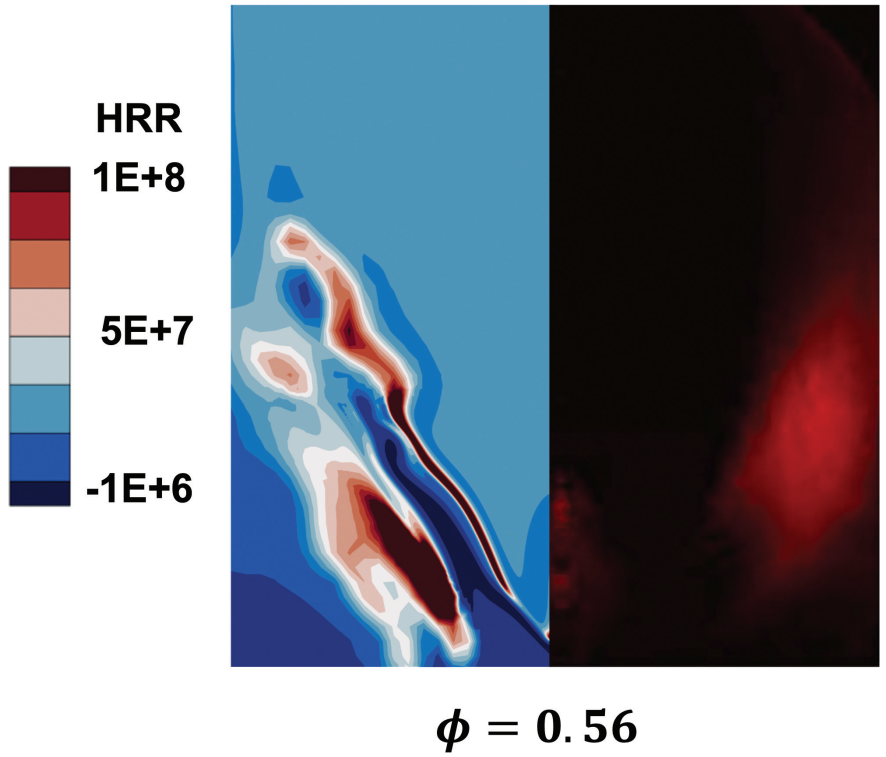


Figure 3.3: Comparison of heat release rate with the OH chemiluminescence image taken from Sidey and Mastorakos 2018.*

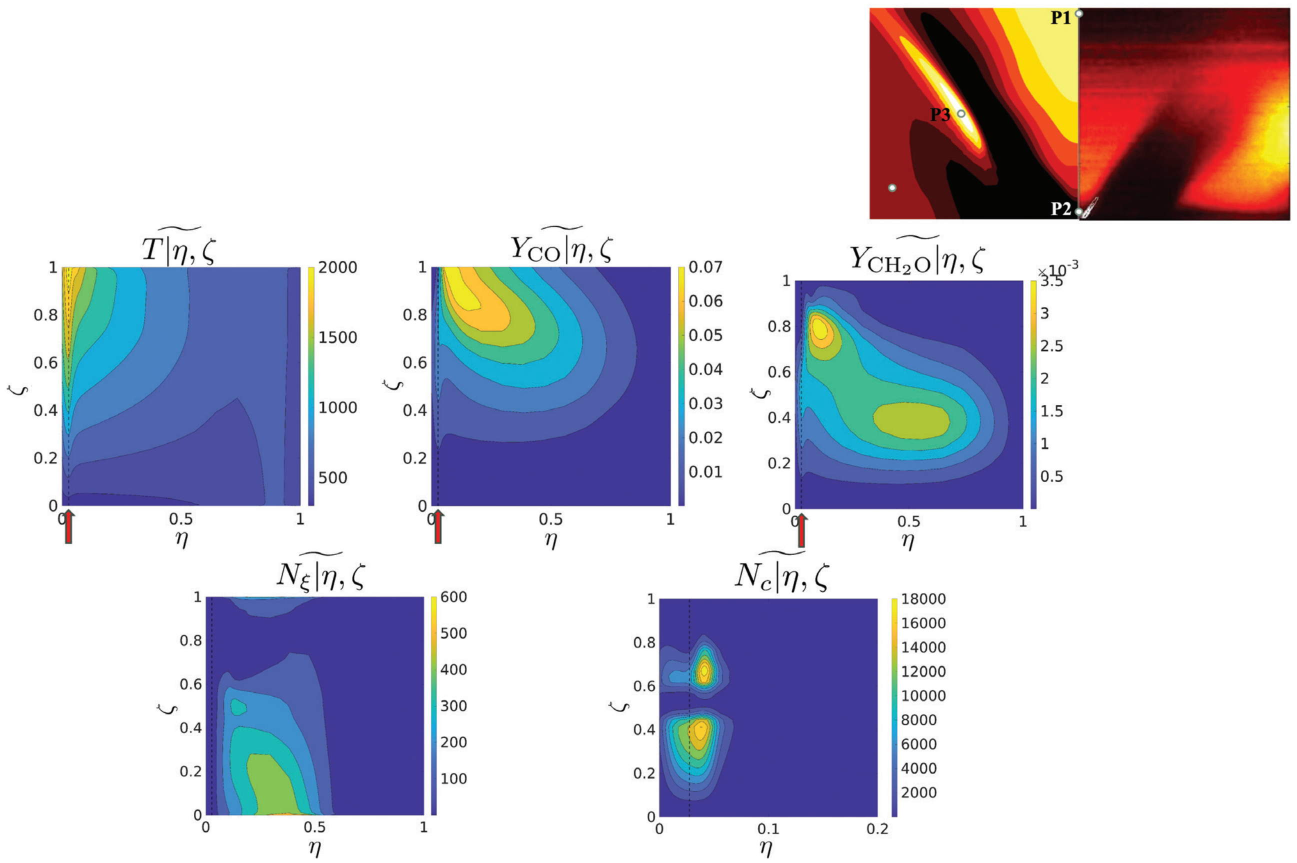


Figure 3.4: Conditional reactive species at a representative point in the domain for premixed equivalence ratio ($\phi_{premixed}$) of 0.56.

CARBON POLICY

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

Principal Investigators

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 decarbonisation pathways for carbon intensive sectors in Singapore. Their study on the evaluation of maritime decarbonisation technologies such as onboard carbon capture systems and zero/near zero maritime fuels establishes a framework for understanding the potential interplay between maritime carbon abatement through clean technology adoption and carbon pricing and the economic impact on downstream commodities. Their findings suggest that under the current literature, onboard carbon capture systems are the cheapest technology option with marginal abatement cost bounds of around 188-199 USD/tCO_2. Furthermore, these bounds are lower than the corresponding thresholds in the proposed GHG pricing mechanism in the IMO Net Zero Framework, implying the potential to induce fleet conversion under clean technology adoption for ship owners subject to this carbon pricing mechanism. An analysis of the downstream economic impact of this pricing mechanism suggests that a flat carbon price could disproportionately affect low-value, high-volume commodities like iron ore and coal, potentially altering their competitive positioning and global trade flows. In contrast, high-value commodities like copper may absorb the additional cost with minimal market disruption. Overall, the price increases resulting from either the imposition of a carbon tax or the adoption of new technologies generally fall within or even below the range of price variations that downstream consumers already experience. Consequently, carbon taxes are likely to function as a marginal cost increase rather than a primary driver of price volatility. Some of these findings have been presented in the SINERGIE 2025 conference held from 29th September to 2nd October 2025 at the NTU Research Techno Plaza in Singapore. The group has also started to utilise this framework to study other carbon intensive sectors such as power, semi-conductors, and oil and gas.

DIGITALISATION

CN23: Introducing next generation laboratory

Principal Investigators

Prof Markus KRAFT (CAM)

During this reporting period, the development and integration of the Digital Laboratory Framework was successfully completed using The World Avatar (TWA). To ensure secure access control, Keycloak was implemented for user authentication and authorisation, while Nginx was configured to support client certificate validation. All framework components were containerised using Docker, making the system platform-independent and readily deployable across diverse servers and laboratory environments. This technical architecture enhances scalability and interoperability—key features for smart laboratories—and has advanced the technology readiness level of TWA through the incorporation of industrial standards.

In parallel, the team developed a proof-of-concept laboratory equipment booking system that interacts with TWA knowledge graph. By dynamically creating and updating instances of laboratory users and resources within the knowledge graph, the system supports more efficient planning, utilisation, and accountability. Figure 4.1 illustrates the user interface of the booking system.

These developments have been presented to industry stakeholders at various events. Feedback from these engagements reaffirmed the value of leveraging TWA knowledge graph to improve system and data interoperability within laboratories.

The work was also presented at the AI4X Conference in Singapore, where a poster based on the paper "The Digital Laboratory Facility Manager: Automating Operations of Research Laboratories through The World Avatar" (DOI: 10.1016/j.ynexs.2024.100031) raised awareness of the initiative within the local research community. The poster was awarded first prize in the AI4X 2025 Poster Presentation Competition. In September 2025, our submission to the IChemE Global Awards 2025, entitled "Revolutionising Laboratory Automation Across Sectors and Regions with The World Avatar", was shortlisted as a finalist.

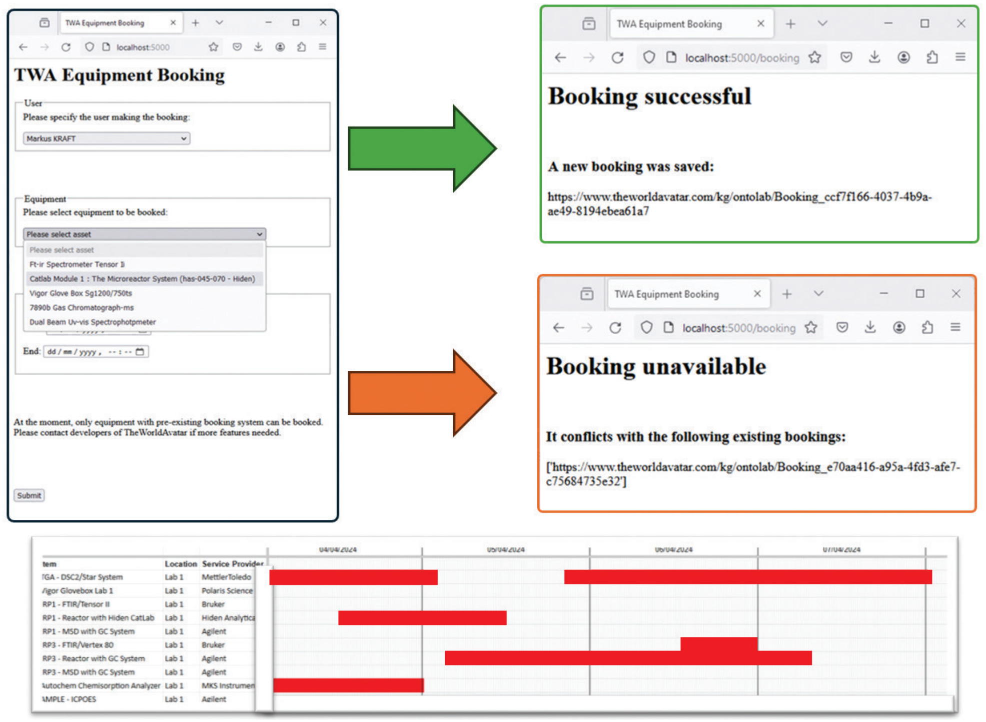


Figure 4.1: User interface of the laboratory equipment booking system.

CN24: Developing the Automated Lab of the Future

Principal Investigators

Prof Markus KRAFT (CAM)

During this reporting period, significant progress has been achieved in both the experimental and computational development of an automated laboratory of the future, with a particular focus on the synthesis and characterisation of Metal-Organic Polyhedra (MOPs).

Firstly, an automated assembler tool was developed to generate accurate MOP structural data from organic and metal molecular subcomponents, combined with a desired assembly model template. The generated structures demonstrated excellent agreement with experimentally reported data.

Secondly, the team showcased the transformative potential of coupling explicit knowledge models with a large language model (LLM)-driven agent within The World Avatar (TWA). This approach enabled the accurate and comprehensive extraction of nearly 300 reported MOP synthesis procedures. Building on this foundation, a reasoning agent was developed that not only assimilates recorded experimental conditions but also extrapolates emerging trends to propose novel synthesis strategies. This advancement extends beyond material discovery to synthesis discovery. Its effectiveness was demonstrated through the successful preparation of three Zirconium-based MOPs (Zr-BDC, Zr-BTC, Zr-BPDC) under conditions proposed by the agent. Powder X-ray diffraction confirmed phase purity and structural fidelity in excellent agreement with literature, demonstrating the agent's ability to accelerate materials discovery and bridge the gap between data-driven inference and experimental realisation.

Thirdly, multi-fidelity simulations were applied to MOP structures, enabling predictions of stability and properties relevant to host–guest applications. These simulations were incorporated into a workflow in which calculation results and parameters are automatically recorded within the knowledge graph, where they can subsequently be queried using natural language.

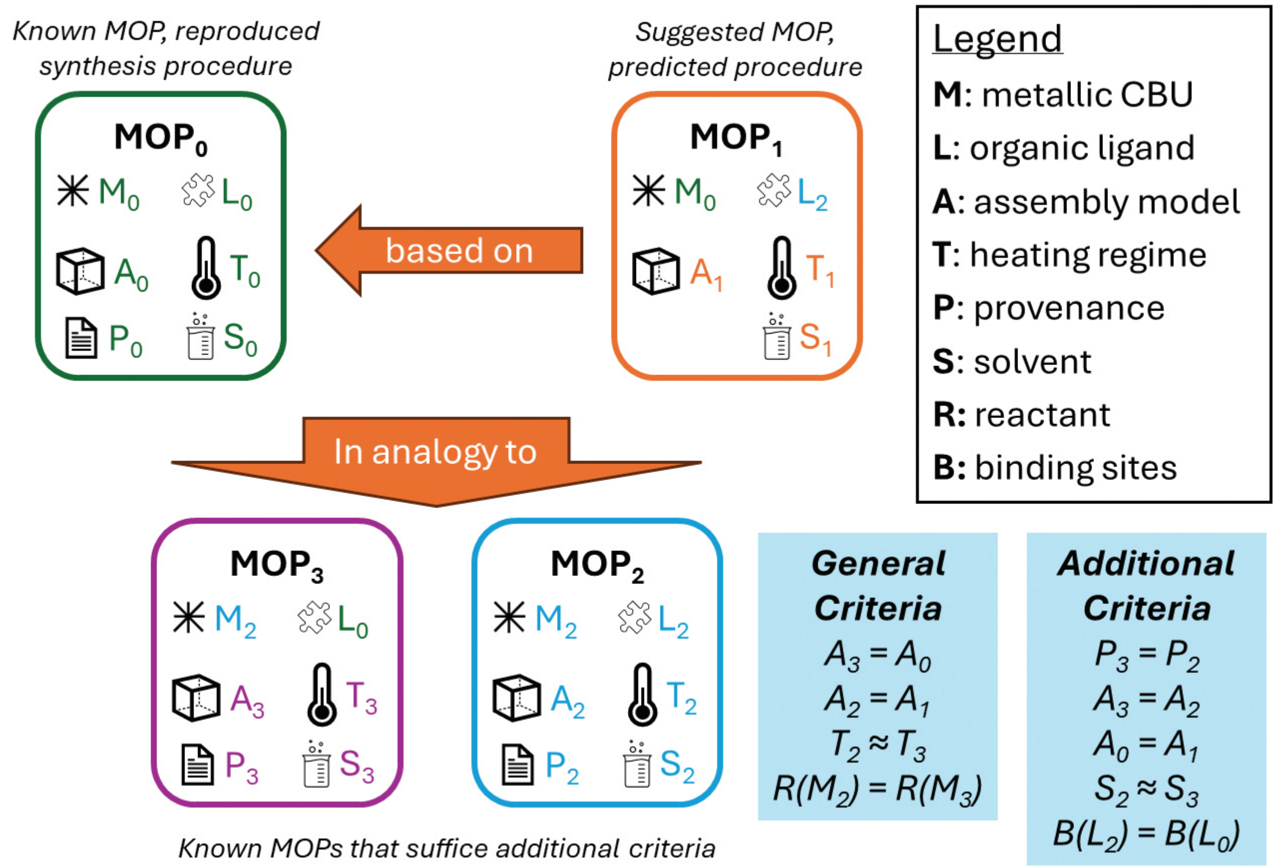


Figure 4.2: Illustration of the rule-based synthesis prediction algorithm for novel MOP structures.

References

Sidey, J. A. M.; Mastorakos, E. Stabilisation of Swirling Dual-Fuel Flames. Experimental Thermal and Fluid Science 2018, 95, **65–72**. https://doi.org/10.1016/j.expthermflusci.2018.02.007.

SCIENTIFIC OUTPUT

The following are the CREATE-acknowledged publications generated by the C4T programme during the reporting period.

Comparative Techno-Economic Analysis of Integrated Process Designs Combining LNG Cold Utilization and Carbon Capture

Ayachi, F.; Law, L. C.; Mastorakos, E.; Romagnoli, A., *Journal of Cleaner Production*

https://doi.org/10.1016/j.jclepro.2025.146274

Twa: The World Avatar Python Package for Dynamic Knowledge Graphs and Its Application in Reticular Chemistry

Bai, J.; Rihm, S. D.; Kondinski, A.; Saluz, F.; Deng, X.; Brownbridge, G.; Mosbach, S.; Akroyd, J.; Kraft, M., *Digital Discovery*

https://doi.org/10.1039/D5DD00069F

Investigating the Kinetics of CO_2 Mineralization via the Carbonation of CaO in Ammonium Carbonate Solution by Reaction Heat Flow Calorimetry

Binte Mohamed, D. K.; Lapkin, A. A.; Wang, C.; Bu, J.; Tao, L.; Liu, W., *Industrial & Engineering Chemistry Research*

https://doi.org/10.1021/acs.iecr.5c01369

Transforming Building Retrofits: Linking Energy, Equity, and Health Insights from The World Avatar

Chen, J.; Bai, J.; Xu, J.; Farazi, F.; Mosbach, S.; Akroyd, J.; Kraft, M., *Advances in Applied Energy*

https://doi.org/10.1016/j.adapen.2025.100230

Question Answering System for Smart Cities and Urban Planning With The World Avatar

Deng, X.; Tsai, Y.; Ganguly, S.; Tran, D.; Quek, H. Y.; Ang, W.; Phua, S. Z.; Mosbach, S.; Akroyd, J.; Kraft, M., *IET Smart Cities*

https://doi.org/10.1049/smc2.70009

Machine Learning-Driven Optimization of Continuous-Flow Photoredox Amine Synthesis

Jorayev, P.; Soritz, S.; Sung, S.; Jeraal, M. I.; Russo, D.; Barthelme, A.; Toussaint, F. C.; Gaunt, M. J.; Lapkin, A. A., *Organic Process Research & Development*

https://doi.org/10.1021/acs.oprd.4c00533

Automated Assembly Modeling of Metal–Organic Polyhedra

Kondinski, A.; Oyarzún-Aravena, A. M.; Rihm, S. D.; Bai, J.; Mosbach, S.; Akroyd, J.; Kraft, M., *European Journal of Inorganic Chemistry*

https://doi.org/10.1002/ejic.202500115

Shape-Selective Molecular Separations Enabled by Rigid and Interconnected Confinements Engineered in Conjugated Microporous Polymer Membranes

Lu, Y.; Deng, H.; Zhang, L.; Wang, Y.; Zhang, S., *Advanced Science*

https://doi.org/10.1002/advs.202416266

Advances in Characterization of Black Carbon Particles and Their Associated Coatings Using the Soot-Particle Aerosol Mass Spectrometer in Singapore, a Complex City Environment

Ma, M.; Rivellini, L.-H.; Zong, Y.; Kraft, M.; Yu, L. E.; Lee, A. K. Y., *Atmospheric Chemistry and Physics*

https://doi.org/10.5194/acp-25-8185-2025

Extraction of Chemical Synthesis Information Using the World Avatar

Rihm, S. D.; Saluz, F.; Kondinski, A.; Bai, J.; Butler, P. W. V.; Mosbach, S.; Akroyd, J.; Kraft, M., *Digital Discovery*

https://doi.org/10.1039/D5DD00183H

Non-Linear Spin Correlation of Intermediates in Enhanced Electrochemical Nitrate Reduction under Magnetic Fields

Shao, D.; Wu, Q.; Zhang, Y.; Cai, X.; Dai, C.; Zhu, S.; Meng, F.; Song, P.; Li, X.; Ren, X.; Wu, T.; Xu, Z. J., *Energy & Environmental Science*

https://doi.org/10.1039/D5EE02132D

Atomically Dispersed Zn and Ir Synergistic Modulation of Substrate and Active Sites for High-Performance Ammonia Oxidation

Shen, Q.; Dai, C.; Liu, Y.; Zhang, Y.; Song, P.; Xi, P.; Xi, S.; Fisher, A. C.; Elouarzaki, K.; Xu, Z. J., *Angewandte Chemie*

https://doi.org/10.1002/ange.202513465

Beyond Connected Digital Twins – Can Digital Twins Really Deliver Sustainable Cities?

Tan, Y. R.; Hofmeister, M.; Phua, S. Z.; Brownbridge, G.; Rustagi, K.; Akroyd, J.; Mosbach, S.; Bhave, A.; Kraft, M., *Sustainable Cities and Society*

https://doi.org/10.1016/j.scs.2025.106596

Municipal Heat Planning within The World Avatar

Tsai, Y.-K.; Hofmeister, M.; Ganguly, S.; Rustagi, K.; Tan, Y. R.; Mosbach, S.; Akroyd, J.; Kraft, M., *Energy and AI*

https://doi.org/10.1016/j.egyai.2025.100479

Efficient Electrocatalytic Nitrate-to-Ammonia Enabled by Reversible Lattice-Oxygen Control

Wu, Q.; Shao, D.; Dai, C.; Wang, J.; Li, X.; Song, P.; Xie, W.; Xi, S.; Zhang, L.; Lin, X.; Luo, S.; Sun, S.; An, L.; Xi, P.; Xu, Z. J., Journal of the American Chemical Society

https://doi.org/10.1021/jacs.5c10362

Minireview on Decoding Electrocatalytic CO_2 Reduction via Lewis Acid-Base Chemistry: Advances and Outlook.

Ye, Y.; Wu, Q.; Xu, Z. J., *Energy Fuels*

https://doi.org/10.1021/acs.energyfuels.5c03374

Cooperative Spin Alignment Enhances Dimerization in the Electrochemical Ammonia Oxidation Reaction

Zhu, S.; Wu, Q.; Dai, C.; Yu, A.; Wu, T.; Ren, X.; Li, X.; Tadich, A.; Deng, D.; Liu, T.; Wu, Q.; Yue, M.; Xu, Z. J., *Nature Chemistry*

https://doi.org/10.1038/s41557-025-01900-1

OTHER ACTIVITIES AND ACHIEVEMENTS

Sustainable Reaction Engineering

CARES team engaged in the CN projects are actively collaborating with the company spun out of CARES in the 2nd phase of the C4T project – Chemical Data Intelligence (CDI) Pte Ltd.

Within CN projects, CDI has assisted CARES in developing the database of renewable resources for decarbonising chemicals value chain, and was supporting collaboration with NUS on developing sustainable chemical pathways to functional molecules.

Dr Zhen Guo and Dr Adarsh Arun became full time employees of CDI from January 2025. In the spring of 2025, Adarsh Arun has successfully defended his PhD.

Electrochemistry

Dr Qikai SHEN (Research Fellow, NTU) presented a poster titled "Unravelling Intrinsic Electronic Factors in Thermocatalytic (Hemi-)Hydrogenation of Ethylene and Acetylene with Electric Polarization" at the Trilateral Conference on Advances in Materials Science (TCAMS 2025) from 24 - 26 March 2025 in Singapore.

Dr Chencheng DAI (Research Fellow, NTU) presented a poster titled "Suppressing product crossover and C–C bond cleavage in a glycerol membrane electrode assembly reformer" at the GLObal Conference for Women Leaders and Emerging Researchers in Materials Science (GLOW) from 29 September - 1 October 2025 in Singapore.

Dr Dai has also filed an international patent application for "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. PCT Application No: PCT/SG2025/050390.

Dr Dai has another patent application "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. The Patent Committee has approved a recommendation to enter the national phase in Europe (EP), Singapore (SG) and the United States (US).

Maritime Decarbonisation

Dr B. HARIKRISHNAN (Research Fellow, CARES) presented the findings "Large eddy simulation of dual-fuel swirl flames" at the 13th Mediterranean Combustion Symposium from 1 – 5 June 2025 in Corfu, Greece. The research showcased the predictive capability of **dcmcConverge** for complex dual-fuel spray combustion.

EMICAST, the spin-off co-founded by Dr Li Chin LAW (Research Fellow, CARES) and Prof Epaminondas MASTORAKOS (PI, CAM), signed an NDA with Value Maritime in November 2024. This was not listed in the previous reporting, hence its inclusion in this report.

Carbon Policy

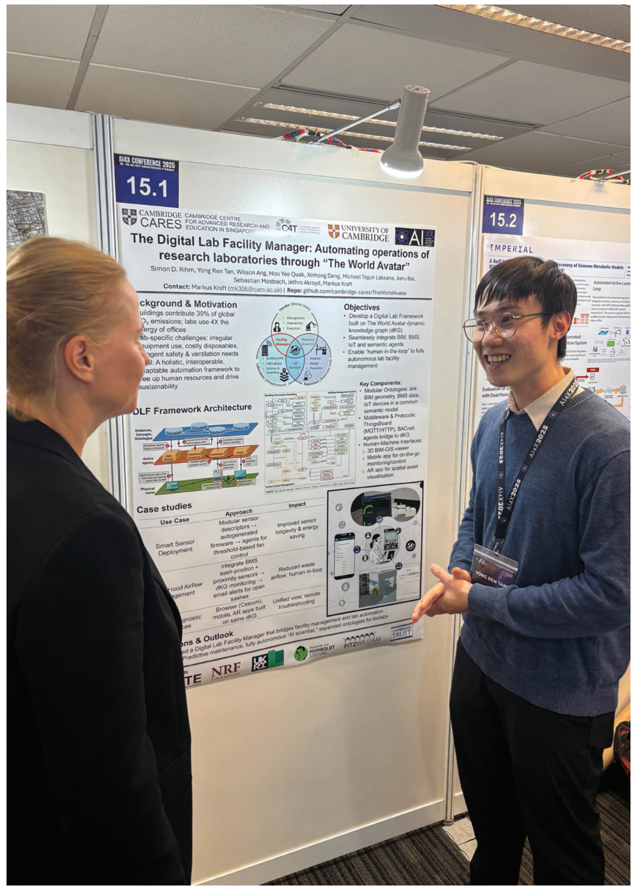
Dr J. Lemuel MARTIN (Research Fellow, NTU) presented "Economics of Maritime Decarbonization: Technologies, Carbon Pricing, and Downstream Impact" at the SINERGIE 2025 conference from 29 September – 2 October 2025 at the NTU Research Techno Plaza in Singapore.

Digitalisation

Dr Yong Ren TAN (Research Fellow (Project Manager), CARES) presented his work at several conferences:

- "Digital Laboratory Framework Powered by The World Avatar" at Singapore AI Research Week on 24 April 2025
- Joined the 2nd Dialogues in APT International Workshop from 26 – 28 May 2025
- "Quantitative Analysis of Soot Formation in PODE3/PODE4-Diesel Blended Flames Using Laser-Induced Incandescence" at the 13th Mediterranean Combustion Symposium in Corfu, Greece from 1 – 5 June 2025
- "The Digital Laboratory Facility Manager: Automating Operations of Research Laboratories through 'The World Avatar'" at the AI4X Conference in Singapore from 8 – 11 July 2025.

Dr Yong Ren Tan (left) and Dr Adarsh Arun (recently completed CARES PhD student) (right) at the AI4X Conference 2025.



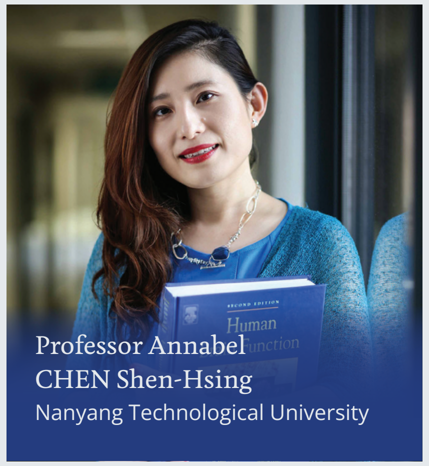
Dr Tan presenting his work at the AI4X Conference 2025.

CLIC

CENTRE FOR LIFELONG LEARNING AND INDIVIDUALISED COGNITION

The Centre for Lifelong Learning and Individualised Cognition (CLIC) is a programme within the Science of Learning initiative, harnessing advancements in neuroscience to develop lifelong learning programs. CLIC is dedicated to enhancing lifelong learning and cognitive flexibility through pioneering interdisciplinary research, with the goal of developing educationally relevant cognitive flexibility paradigms that inform future interventions across the lifespan.

Directors



Professor Annabel CHEN Shen-Hsing
Nanyang Technological University

Professor Zoe KOURTZI
University of Cambridge

This reporting period marked an exciting phase of growth and progress across CLIC's three Work Packages. **Work Package 1 (SLiCX intervention)** reached new milestones with enhanced task complexity, gamified elements, and active control conditions. The team successfully launched its first pilot studies and neuroimaging protocols, while early findings from the infant creativity pilots revealed promising connections between creativity and cognitive flexibility. **Work Package 2** made steady strides, completing pre-tests with 58 participants in its language-learning study exploring how multilingualism shapes cognitive flexibility. **Work Package 3** advanced with pilots of *Crossing Valley* alongside the Singapore Examinations and Assessment Board's (SEAB) Critical, Analytical, and Inventive Thinking (CAIT) task, with close collaborations with the Ministry of Education to ensure the research translates meaningfully into classroom practice.

At the **Scientific Advisory Committee (SAC) review** on 29 July 2025, the committee commended CLIC's strong progress and interdisciplinary integration. The SAC encouraged the team to further highlight CLIC's role in preparing Singapore's education system and workforce for technological change and pedagogical innovation. The team is actively pursuing SAC's recommendations.

CLIC also had public and academic engagements. During the **Curious Worlds Festival** (April 2025) at the ArtScience Museum, Profs Annabel Chen and Henriëtte Hendriks engaged audiences with a talk on the brain, learning, and flexibility, accompanied by an interactive booth offering hands-on experiences with neuroimaging technologies. In **September 2025**, CLIC's Principal Investigators and Research Fellows convened in Cambridge for a dynamic week of strategic meetings, research collaborations, and participation in the 8th Cambridge Neuroscience Symposium. The highlight was the flagship event **Enhancing Cognitive Flexibility: CLIC(k)ing into Lifelong Learning**, featuring workshops, panel discussions, and cross-disciplinary exchanges that reinforced CLIC's role in connecting research, education, and policy. We were delighted to have both the Vice-Chancellor of the University of Cambridge, Prof Deborah Prentice, and the Pro-Vice-Chancellor for Research, Prof Sir John Aston, attend our flagship event in Cambridge.

To nurture talent and collaboration, CLIC launched a monthly **Brown Bag Series** in May 2025, creating a lively platform for Research Fellows to share insights and develop new skills. These sessions which were also open to the wider CARES and CREATE communities, have become a hub for mentorship, dialogue, and idea exchange.

CLIC's outreach and influence continue to grow both locally and globally. Prof Hendriks shared insights on multilingualism and cognitive flexibility with CREATE, CARES, and CRADLE@NTU audiences; Prof Chen inspired educators at the National Teachers' Conference and ExCEL Fest 2025; and Prof Trevor Robbins delivered keynote lectures in Beijing and London. Together, these efforts showcase CLIC's momentum in advancing the science of learning and translating research into real-world impact.

Looking ahead, CLIC is poised to build on this momentum and deepen its impact across research, education, and policy. The coming year will see the expansion of pilot studies and strengthened partnerships with educational stakeholders. Through these efforts, CLIC aims to translate its scientific discoveries into meaningful learning innovations that empower individuals, enrich teaching practices, and equip Singapore's learners to thrive in an ever-changing world.

Professor Annabel Chen Shen-Hsing
Director of CLIC, NTU

Professor Zoe Kourtzi
Director of CLIC, CAMBRIDGE

WORK PACKAGE 1

The Structure Learning-based Cognitive Flexibility Training Suite (SLiCX) intervention is progressing well for implementation in Phase 2. The updated Structure Learning (SL) training incorporates new dimensions to enhance task complexity and fit for both shifting (CF1) and strategy flexibility (CF2). Additionally, three pilot studies have been designed to assess salience, evaluate different contingencies and progression criteria across the adult and adolescent populations. Piloting of SLiCX parameters for adults is completed as of September 2025. While recruitment for adolescent participants has been a challenge, the team are planning several outreach events and opportunities at local schools to build a strong recruitment network ahead of the main study.

In line with recommendations from the Scientific Advisory Committee (SAC), a gamified version of the SL task to improve engagement and motivation in participants is being developed. Significant headway is expected as technical challenges (i.e., delays in the iABC server set-up in Cambridge) has been resolved, enabling seamless integration of SLiCX development within the platform. Building on the SAC's advice to include an explicit training arm, the team has adopted All You Can ET (AYCET), a validated set-shifting paradigm developed by the NYU-CREATE Lab, to serve as an active control to the implicit SL training. This collaboration allows for a direct and theoretically grounded basis for comparison between two distinct forms of cognitive flexibility training. In addition to the development of the SLiCX platform, the cognitive task batteries and protocols are finalised for implementation in Phase 2. Significant progress has also been made in coordinating the technical setup of these tasks, including detailed testing of the AYCET task to ensure technical issues are resolved and ensure task readiness for deployment.

Protocols for neuroimaging data collection have been refined based on findings from Phase 1. These include non-verbal instructions, nature visuals, and embedding the Structure Learning task within both pre- and post- training scans to capture associated neuronal changes. The optimised multi-modal imaging protocol now integrates structural, magnetic resonance spectroscopy, quantitative multi-parametric mapping, resting-state function MRI, and diffusion spectrum imaging within a streamlined 90-minute session. Imaging analysis pipelines have also been strengthened through collaborations with Prof Zoe KOURTZI (PI & Co-Director, CAM) and her lab in Cambridge. Neuroimaging pilots for both adults and adolescents are close to completion. The team is currently working on multimodal data quality assessments along with development of streamlined data analysis pipelines for Phase 2.

Beyond SLiCX, the team continues to deepen CLIC's understanding of cognitive flexibility and creativity across the lifespan with significant progress made in the infant study. Pilot testing with infants aged between 12-36 months have revealed promising links between creativity and emerging cognitive flexibility skills such as attention and strategy shifting. The team aims to examine the neural and physiological mechanisms underpinning these relationships along with social moderators of parent-child interaction in the next phase of the study. The upcoming study will integrate EEG, ECG, and neuromodulation methods to examine underlying neural and physiological mechanisms.

WORK PACKAGE 2

Steady progress has been made across several ongoing intervention studies investigating language learning, social framing, and career development.

Language Learning Study

Data collection is in progress, with 54 adult participants recruited to date.

Social Framing Study

This study investigates how cooperative and competitive social framing influences task performance within a structure-learning paradigm, and how these effects are moderated by individual differences in trait social orientation. The experimental design, including tasks and questionnaires, has been finalised, and preparation of the Institutional Review Board (IRB) protocol is currently underway.

Career Study

Advances have been made in developing the intervention design and questionnaires aimed at examining how cognitive flexibility, career adaptability, and related competencies influence decision-making. The research design continues to be refined through ongoing literature review and conceptual development. In August, preliminary findings on career adaptability and cognitive flexibility were presented to SkillsFuture Singapore (SSG), whose feedback will inform data analysis and guide the next phase of the study.

Significant research outputs have also been achieved. A paper titled "Validation of the CILD-Q for Measuring Contextual Linguistic Diversity in Singapore" (Melia et al., 2025) has been accepted for publication in the International Journal of Multilingualism. Collaboration with Work Package 3 is underway on a manuscript examining the relationship between multilingualism and cognitive flexibility across adolescent and adult populations.

In September 2025, a poster titled "QualGames: A Qualtrics Implementation and Database of Behavioural Game Theory Tasks" was presented by Dr Shengchuang FENG (Research Fellow, NTU) at the 8th Cambridge Neuroscience Symposium. Four additional manuscripts on decision-making and personality are being developed, addressing behavioural game theory tasks, measurement issues in the Big Five Inventory, language entropy and cooperativeness, and the association between receptiveness to opposing views and trust.

Further progress has been made on two career-focused manuscripts: one evaluating the Career Construction Model of Adaptation (CCMA; Savickas & Porfeli, 2012), and another examining how cognitive flexibility moderates the relationship between career adaptation dimensions and income among working adults in Singapore.

WORK PACKAGE 3

Work Package 3 focuses on translating CLIC's research findings into authentic classroom, problem-solving, and practice contexts. During this reporting period, continued collaboration with the Singapore Examinations and Assessment Board (SEAB) has been maintained to validate SEAB's Critical, Analytical, and Inventive Thinking (CAIT) assessment against CLIC's cognitive flexibility indices.

In May 2025, a large-scale data collection was conducted across four secondary schools, involving over 150 participants and supported by researchers across multiple work packages. In parallel, *Crossing Valley*, a serious game integrating cognitive flexibility and creativity principles into a problem-solving context, was successfully piloted. The game introduces uncertainty and resource constraints that mirrors lab-based tasks, enabling the observation of CF2 (Strategy Flexibility) in a simulated real-world context. Approximately 70 adolescents from a local secondary school participated in the pilot, and exploratory data analyses are underway to derive key metrics related to cognitive flexibility and other executive functions from gameplay data.

In July 2025, a follow-up meeting with SEAB was had to review progress and plan subsequent steps for the CLIC–SEAB collaboration. This discussion enhanced mutual understanding of SEAB's CAIT scoring framework and identified opportunities for integrating CLIC's cognitive flexibility research into future task design and analytical approaches.

Building on the applied studies, several manuscripts and projects are progressing toward publication and implementation. These include a study examining the relationship between cognitive flexibility and creativity in adolescents, a validation manuscript for the Contextual Linguistic Profile Questionnaire (CLiP-Q), and an investigation into how intelligence and executive functions influence explanatory coexistence in science learning.

At the international level, Dr Rui WANG (Research Fellow, NTU) participated as a symposium speaker at the European Science Education Research Association (ESERA) Conference 2025 in Copenhagen in August this year. She presented findings from her collaborative research with Prof Michelle ELLEFSON (PI, CAM) on the Explanatory Coexistence of naïve scientific thinking and formal scientific knowledge.

In alignment with recommendations from National Research Foundation (NRF) and the Scientific Advisory Committee (SAC), quarterly meetings will be held with Dr Laik Woon TEH (Ministry of Education) to facilitate the translation of research findings into educational practice. These initiatives ensure that WP3 outputs remain scientifically grounded, policy-relevant, and pedagogically impactful.

SCIENTIFIC OUTPUT

The following are the CREATE-acknowledged publications generated by the CLIC programme during the reporting period.

Validation of the CILD-Q for measuring contextual linguistic diversity in Singapore

Melia, N.; Christopoulos, G.; Wigdorowitz, M.; Vassiliu, C.; Feng, S.; Abraham, A.; Chan, Y. N.; Lee, L. L.; Yap, H. S.; Robbins, T.; Sahakian, B.; Kourtzi, Z.; Leung, V.; Cheng, A.; Hendriks, H.; the CLIC Phase 1 Consortium., ***International Journal of Multilingualism***

https://doi.org/10.1080/14790718.2025.2570205

OTHER ACTIVITIES AND ACHIEVEMENTS

CLIC actively strengthened its public engagement through participation in the Curious Worlds Festival at the ArtScience Museum. Prof Annabel CHEN (PI & Co-Director, NTU) and Prof Henriëtte HENDRIKS (PI & Deputy Director, CAM) delivered public talks on the brain, learning, and cognitive flexibility, while an interactive CLIC booth offered attendees an immersive experience exploring brain imaging technologies such as MRI. The initiative attracted over 420 attendees, demonstrating strong public interest in CLIC's work.

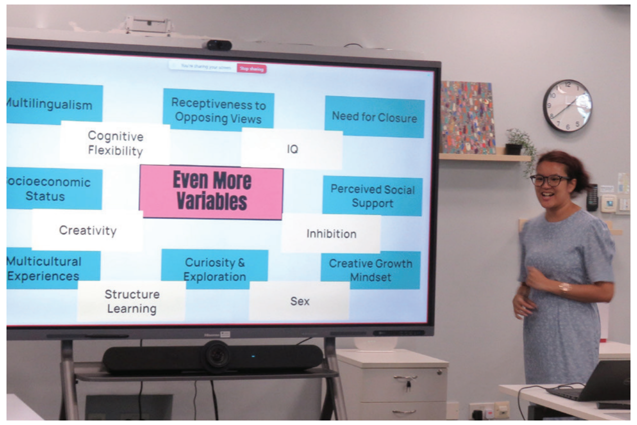
Prof Annabel Chen presenting at the Curious Worlds Festival.

In May 2025, CLIC launched a monthly Brown Bag Session series to promote knowledge sharing and professional development among Research Fellows and junior researchers. Sessions have featured discussions led by Dr Rui WANG (Research Fellow, NTU) on scientific thinking and Dr Nadhilla Velda MELIA (Research Fellow, NTU) on moderation analysis. These sessions are also open to members of the broader CARES and CREATE communities, fostering collaboration, and skill development across research teams.

The CLIC team testing their brain imaging technologies before showcasing it to attendees.

Building on its commitment to bridge research and practice, CLIC has continued to engage with academic and educational communities through invited talks and seminars. Prof Hendriks presented "The Language Factor in the CLIC Project: Multilingualism and Cognitive Flexibility" at CREATE, drawing participants from CARES, CRADLE@NTU, and other CREATE entities. In addition, Prof Chen was invited to speak at the Teachers' Conference and ExCEL Fest 2025 (TCEF2025), a major national platform for educators, further reinforcing CLIC's role in translating neuroscience insights into educational practice.

Dr Rui Wang presenting "Insights from the Naive Thinking Task".



Dr Nadhilla Velda Melia presenting "Analysing sociocognitive variables: A lesson on moderation in R".

In September 2025, CLIC PIs and Research Fellows convened at the University of Cambridge for a series of strategic and research-focused engagements. Activities included participation in the 8th Cambridge Neuroscience Symposium, a meeting to review progress on deliverables and milestones, and the formulation of action plans to advance ongoing research goals.

The visit culminated in CLIC's flagship event in Cambridge, Enhancing Cognitive Flexibility: CLIC(k)ing into Lifelong Learning, which featured workshops in the afternoon divided into three parallel tracks: Early childhood, Adolescence, and Being an adult in a rapidly changing world. For the evening reception, CLIC invited Dr Sao-Ee GOH from the Ministry of Education to join a panel discussion wrapping up the three afternoon themes and offering his perspective on how agencies should be developing policies with researchers. Equally humbling was the chance to have the Vice-Chancellor of the University of Cambridge, Prof Deborah Prentice, and the Pro-Vice-Chancellor for Research, Prof Sir John Aston, providing the opening and closing words for the event respectively.

CLIC's international visibility was further enhanced through two invited keynote lectures by Prof Trevor ROBBINS (Senior Scientific Advisor, CAM) that featured CLIC's research. These included "Fronto-Executive Function: Fractionating Cognitive Flexibility" at Peking University (April 2025) and "The Role of Cognitive Flexibility in Decision-Making – in Health and Disorder" at the British Neuropsychological Society, London (May 2025).

Top: Photos from the afternoon workshops. Bottom: Photo from the evening reception.

Prof Trevor Robbins presenting in the evening reception of CLIC's flagship event in Cambridge

The conference presentations by CLIC are listed below:

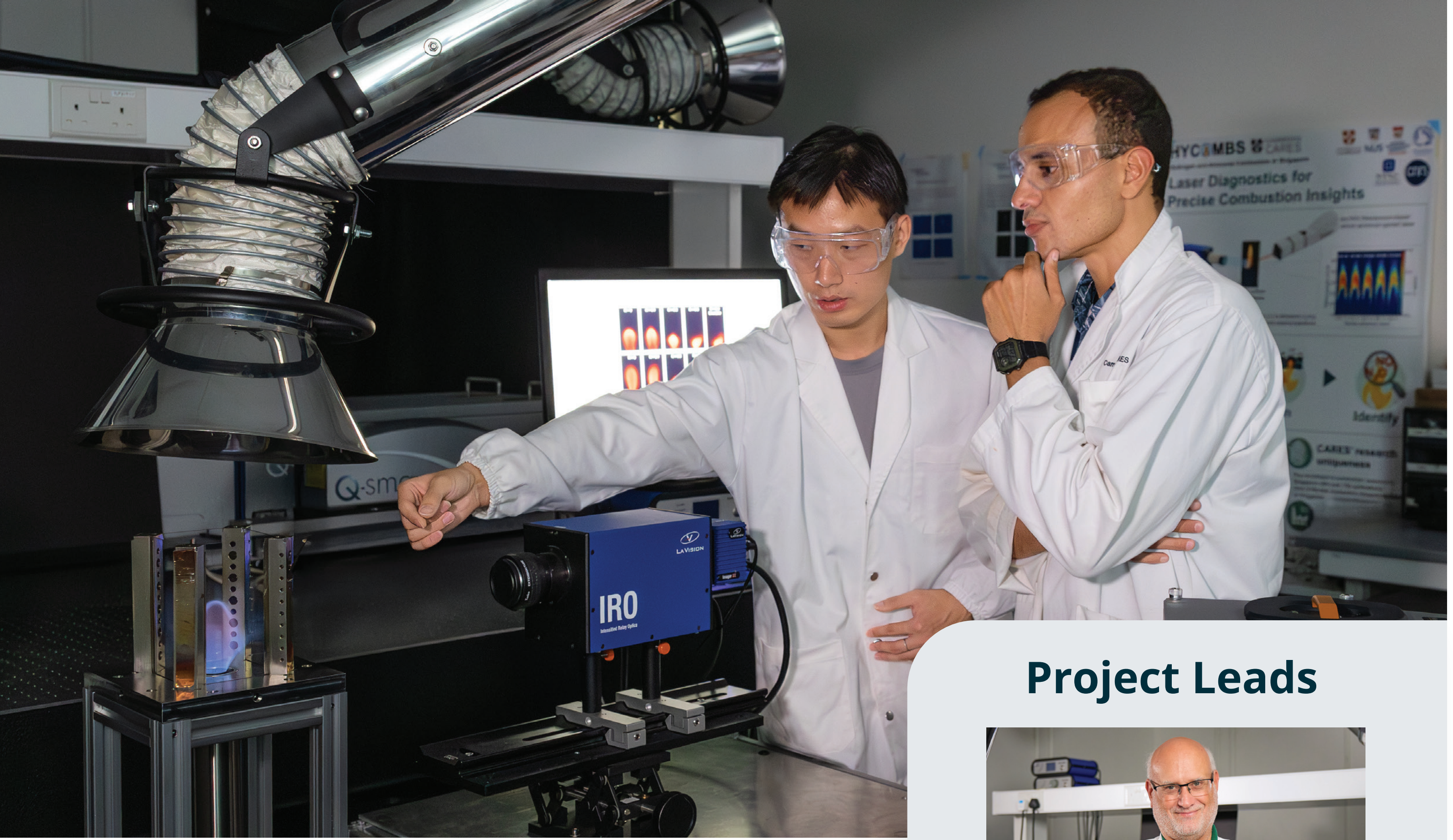
- Dr Deepika SHUKLA (Research Fellow, CARES) presented "Neurochemical (GABA and Glu) cognitive dynamics and myelination in cognitive flexibility" at the Annual Meeting of the Organization for Human Brain Mapping from 24 – 28 June 2025 in Brisbane, Australia.
- Dr Shengchuang FENG (Research Fellow, CARES) presented "QualGames: A database and a Qualtrics implementation of behavioral game theory tasks" at the 8th Cambridge Neuroscience Symposium from 10 – 11 September 2025 in Cambridge, UK.
- Dr Rui WANG (Research Fellow, CARES) presented "Cognitive Flexibility and Inhibition Predict Explanatory Coexistence" at the 8th Cambridge Neuroscience Symposium from 10 – 11 September 2025 in Cambridge, UK.
- Dr Xinchen FU (Research Fellow, CARES) presented "Infant Exploration-Exploitation Behaviour and Developing Cognitive Flexibility in relation to Partner Familiarity" at the 8th Cambridge Neuroscience Symposium from 10 – 11 September 2025 in Cambridge, UK.
- Dr Deepika SHUKLA (Research Fellow, CARES) presented "Cognitive Strategy Flexibility Linked to DLPFC Inhibitory Plasticity" at the 8th Cambridge Neuroscience Symposium from 10 – 11 September 2025 in Cambridge, UK.

Collectively, these initiatives emphasises CLIC's growing scientific credibility, policy relevance, and national and international impact, reflecting steady progress in advancing the science of learning through research, outreach, and collaboration.

CLIC also has various industry engagements:

- Prof Annabel CHEN (PI & Co-Director, NTU) is leading discussions with NYU-CREATE lab (New York University-Consortium for Research and Evaluation of Advanced Technologies in Education) to adopt their set-shifting training paradigm into CLIC's SLiCX intervention for the Active Control Group.
- Assoc Prof Georgios CHRISTOPOULOS (PI, NTU) is leading early-stage discussions with SkillsFuture Singapore to incorporate CLIC's research into the agency's work.

Panel discussion during CLIC's flagship event in Cambridge. From left to right: Dr Goh Sao-Ee, Prof David Hung, Prof Trevor Robbins, Prof Barbara Sahakian, and Prof Victoria Leong.



HYCOMBS

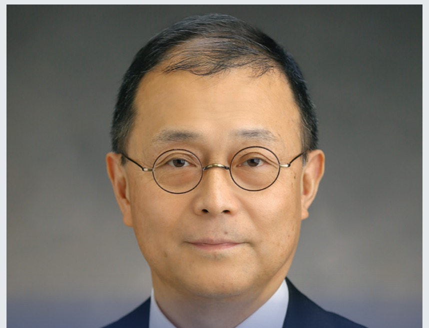
HYDROGEN AND AMMONIA COMBUSTION IN SINGAPORE

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.

Project Leads

Professor Epaminondas MASTORAKOS
University of Cambridge

Assoc Professor Fei DUAN
Nanyang Technological University



Professor Kaoru MARUTA
Tohoku University

In this reporting period, significant progress has been achieved in expanding the research team, with 12 new Research Fellows (RFs) appointed and now actively contributing to HYCOMBS research activities. An additional three RFs are expected to begin in Q4 2025.

Hydrogen (H_2)-based combustion experiments have commenced using the newly completed Swirl burner rig, building on CARES laboratory's existing H_2 research infrastructure (more details in the WP2 section). For ammonia (NH_3)-based combustion experiments, additional infrastructure development is underway. It will incorporate critical components such as NH_3 gas cylinders, distribution piping networks, specialised gas detection sensors, and containment mechanisms. They are essential for regulatory compliance and safe experimental operations.

Another notable mention was that the project team successfully showcased key HYCOMBS research objectives during the visit of Mr Tharman Shanmugaratnam, President of the Republic of Singapore, to the CARES laboratory on 8 July 2025. This high-level engagement highlighted Singapore's commitment to advancing clean combustion technologies and enhanced project visibility.

Additionally, the team participated in Singapore Maritime Week 2025 in March 2025, strengthening ties with potential industrial partners in the maritime sector. Prof Epaminondas MASTORAKOS (Programme Lead, CAM) and Prof Christine ROUSELLE (PI, CNRS) delivered a talk on "Bridging university R&D with the maritime industry," discussing pathways to advance R&D to higher TRLs from both academic and industry perspectives.

Top: President Tharman Shanmugaratnam's visit to the CARES laboratory. Bottom: CARES at Singapore Maritime Week 2025.

WP1: CHEMICAL KINETICS

Progress has been made in two key activities related to chemical kinetics over the past six months. Firstly, for the micro flow reactor (MFR) development, components for the MFR rig have been procured, and the gas chromatography-mass spectroscopy (GCMS) system is on track for full commissioning in Q4 2025. Arrangements are also underway to use the high-pressure rig in Tohoku.

For the plasma interaction studies, the work on studying plasma interactions has begun. A connection between the plasma generator and the RQL (Rich-Quench-Lean) combustor was designed, with probes positioned diagonally through holes in the burner's corner rod. Preliminary tests confirm the plasma generator system is functioning effectively. A low-cost spectrometer has been purchased to analyse radicals produced by the plasma. Future tests will involve evaluating the system under constant equivalence ratios and bulk velocities using fuels such as NH_3, H_2, and mixtures of the two. An intensified charge coupled device (CCD) camera equipped with filters will also be deployed to capture time-resolved radical emissions from the discharge. This work aims to explore relationships between plasma conditions, their characteristic timescales, and combustion chemistry initiation.

WP2: FLAMES

In this work package, significant progress has been made in understanding flame dynamics and combustion characteristics for NH_3-based and H_2-based fuel systems. The research focuses on laminar and turbulent flame experiments, supported by modelling activities to enhance predictive capabilities for H_2 and NH_3 combustion.

For the laminar flame experiments, the team has completed the design of a specialised laminar flame burner for NH_3 and H_2 combustion studies, with fabrication currently underway. The burner will enable systematic investigations into flame propagation, heat release, and radical production under controlled conditions. In parallel, a postdoctoral researcher joined the team on September 1 2025 to advance laser diagnostics in laminar flames. The researcher will be trained on laser absorption techniques and experimental protocols on a diffusion flame test rig to integrate a tuneable diode laser absorption spectroscopy system. This setup will provide hands-on experience in optical alignment, data acquisition, and temperature measurements, laying the groundwork for future flame characterisation studies.

For the turbulent flame studies, significant progress has been made in investigating lean blow-off (LBO) limits, emissions, and flame stabilisation in turbulent flames using H_2-enriched fuel blends. Experiments conducted on a (high) Swirl burner revealed that H_2 addition lowers the equivalence ratio (ϕ) at which flames blow out, enhancing stabilisation compared to pure CH_4-air flames. The LBO curves of premixed methane (CH_4)-air flames and CH_4/H_2-air flames under various bulk velocities (U) and ϕ are shown in Figure 5.1. The LBO velocities increase linearly with ϕ. Moreover, with the addition of H_2 into the fuel blends, the flames blow out at a lower ϕ at the same U compared with pure premixed CH_4-air flames. Notably, the premixed CH_4-air flames with non-premixed H_2 will not extinguish even when the CH_4 concentration decreases to zero, which demonstrates the stabilisation effect of H_2.

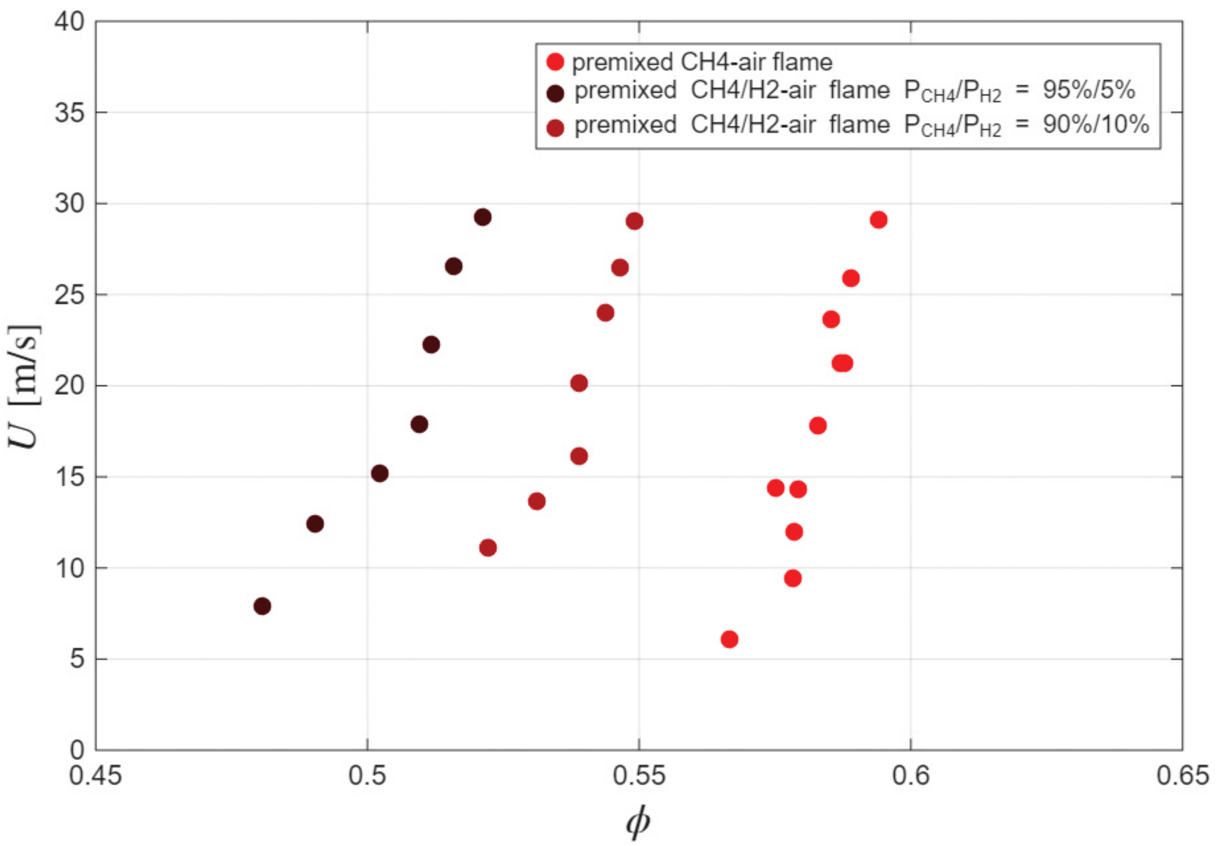


Figure 5.1: Lean blow-off (LBO) curves of premixed CH_4-air flames and premixed CH_4/H_2-air flames under various bulk velocities and equivalence ratios (ϕ).

Chemiluminescence imaging (Figure 5.2) further demonstrated that OH* radicals are distributed more broadly in H_2-enriched flames, contributing to their stability. Compared with premixed CH_4-air flames, in which OH* radicals are concentrated at the end of the inner recirculation zone, OH* radicals are distributed along the shear layer region when non-premixed H_2 is added. Moreover, the flames become shorter with the addition of non-premixed H_2. This might be caused by the fast diffusivity and consumption rates of H_2 which can make the flame more stable. These findings provide critical insights for optimising fuel mixtures in practical energy systems.

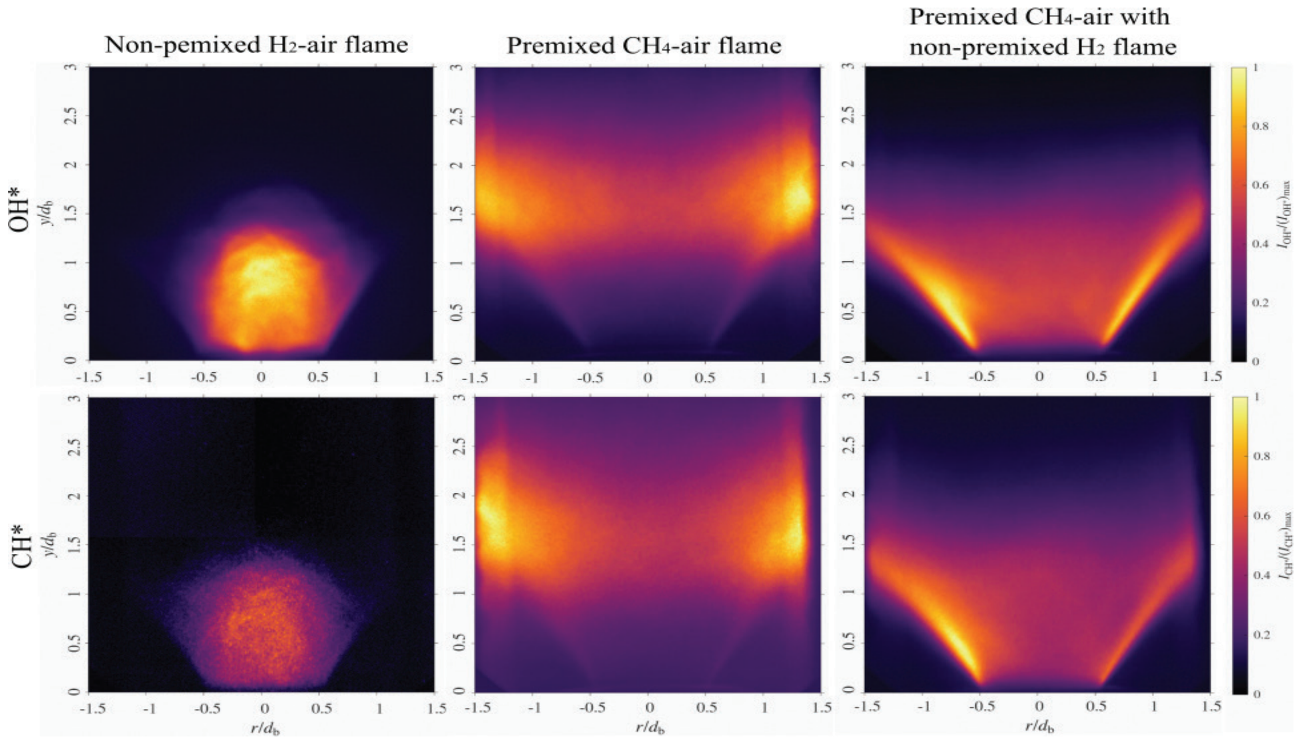


Figure 5.2: Normalised time averaged OH and CH* chemiluminescence images of non-premixed H_2-air flames, premixed CH_4-air flames and premixed CH_4-air with non-premixed H_2 flames. The equivalence ratio for premixed CH_4-air flame is 0.8. The bulk velocity is maintained at 10 m/s for CH_4 flames and at 5 m/s for H_2 flames.*

The team is also advancing optical diagnostics capabilities, including particle image velocimetry (PIV) and planar laser-induced fluorescence, to study species distribution (e.g., NH*, NO) and flame dynamics. Notably, using the same burner, the AC arc plasma will also be applied here to stabilise NH_3-air flames. A range of frequencies and the voltages will be tested on these flames. Both premixed and non-premixed NH_3-air flames, as well as mixtures blended with other fuels such as H_2 and hydrocarbon fuels, will be examined under plasma-assisted conditions. The flame structure, stability limits and thermoacoustic instabilities under these cases will also be studied. A traditional spark ignition and plasma discharges will be compared from the perspective of igniting low-reactivity fuels such as NH_3.

For modelling research activities, computational efforts have focused on developing predictive frameworks for turbulent and laminar flames. Initial groundwork for Large-Eddy Simulation (LES) of the Swirl Burner (turbulent flame) has commenced, including geometry reconstruction, mesh optimisation, and validation of cold-flow simulations using initially RANS and subsequently LES. These simulations will eventually incorporate combustion to investigate flame stabilisation and pollutant formation under different fuelling strategies. These simulations were systematically compared with previously obtained experimental data. This stage helped refine the problem setup, validate the boundary and initial conditions, and highlight the limitations of turbulence models in this configuration. Figure 5.3 presents a comparative analysis between the mean axial velocity fields (U_z) obtained from LES and experimental PIV measurements for the non-reacting flow configuration of the swirl burner. The LES results, shown on the left, represent the preliminary cold-flow solution, with the axial velocity field non-dimensionalised using the bulk velocity (U_b) at the bluff body exit plane. These numerical predictions are directly compared with the corresponding experimentally measured mean axial velocity field, shown on the right, which has been processed and non-dimensionalised in an equivalent manner to ensure consistency. The comparison allows for an assessment of the predictive capability of the numerical framework in capturing key flow features such as radial expansion, recirculation structures, and shear layer development in highly swirling flows. With the cold-flow LES validated, the next phase will focus on hot-flow simulations with combustion, to investigate flame stabilisation, heat release, and pollutant formation under different fuelling strategies.

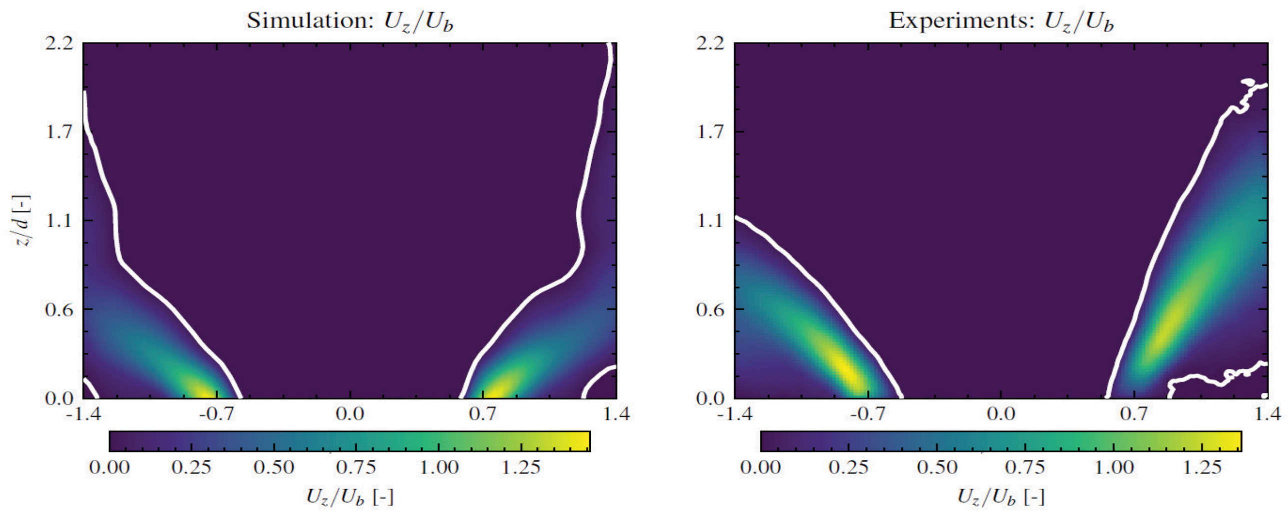


Figure 5.3: Comparison of non-dimensional mean axial velocity fields U_z : (left) preliminary LES cold-flow prediction scaled by bulk velocity U_b, and (right) corresponding PIV measurements under identical conditions.

A complementary study on the chemical kinetics of NH_3/H_2 flames has begun, exploring how H_2 enrichment modifies flame structure, heat release, and radical production. Specifically, the primary interest is the shift of the heat release rate (HRR) peak with varying H_2 content, identifying the radicals most involved, and determining which reactions compete as the H_2 fraction increases. Mixtures of NH_3/H_2 with volumetric H_2 fractions of 0%, 25%, 50%, 75%, and 100% have been considered at operating conditions relevant to domestic and industrial applications (i.e., Pressure, P = 1 bar, Temperature, T = 300 K). Results from detailed chemistry simulations using Cantera provide insights into dominant reaction pathways and radical interactions, forming the basis for reduced-order models and high-fidelity flame simulations. Figure 5.4, as example, illustrates the dominant one-way chemical reaction pathway for an NH_3/H_2/Air premixed flame at an equivalence ratio of ϕ = 0.6 and atmospheric pressure. The pathway is extracted at the location corresponding to the peak heat release rate (HRR), where chemical activity is maximal and the interplay between ammonia and hydrogen oxidation is most pronounced. This representation highlights the primary fuel consumption routes and intermediate species formation, providing insight into the key kinetic mechanisms that govern flame stabilisation and pollutant formation under lean operating conditions.

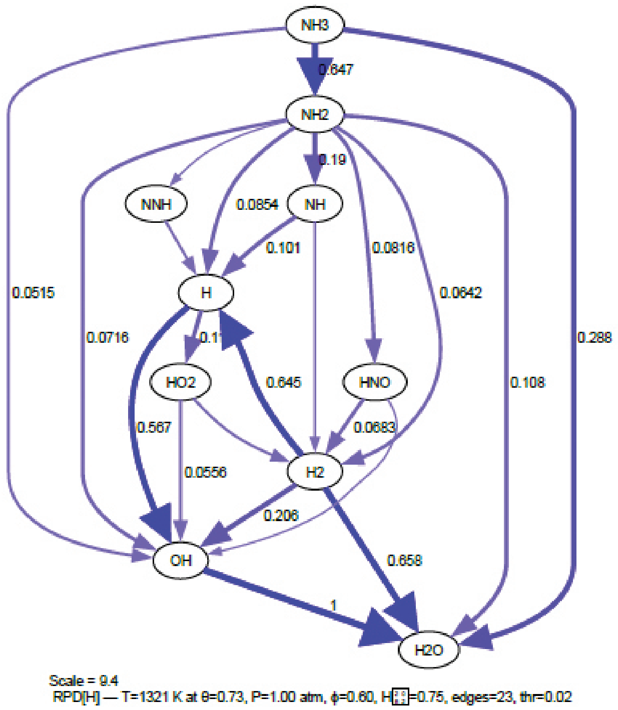


Figure 5.4: One-way kinetic reaction pathway for an $NH_3/H_2/$ air premixed flame at equivalence ratio (ϕ) =0.6 and pressure (P) = 1 atm, evaluated at the location of maximum heat release rate (HRR).

WP3: NOVEL COMBUSTION SYSTEMS FOR GAS TURBINES

Significant progress has been made in advancing the novel combustion systems for gas turbines. Preliminary design work for a new experimental combustion setup has been completed. This setup will support staged operation, independent acoustic excitation of primary and secondary stages, and plasma discharge. Detailed design drawings and manufacturing will proceed in the next phase of the project.

Work has also begun to upgrade infrastructure in the laser lab. This includes ordering equipment such as microphones, amplifiers, mass flow controllers, digital acquisition systems, photomultiplier tubes, cameras, and PIV equipment. Preliminary testing of the mass flow controllers and digital acquisition systems has been conducted to ensure readiness for future experiments.

Additionally, analysis of previously collected data from an axially staged combustion system has commenced. This work focuses on understanding the timescales of HRR oscillations in both the primary and secondary stages and exploring methods to suppress instability. These insights will inform the design of the new experimental setup and guide further data collection. If the analysis yields noteworthy results, it will be submitted to the International Symposium on Combustion 2026.

WP4: NOVEL COMBUSTION SYSTEMS FOR RECIPROCATING ENGINES

The understanding of flame structure, ignition behaviour, and combustion kinetics for H_2, NH_3 and their blends remains a critical research priority for reciprocating engine applications. Progress in this area has relied heavily on experimental tools capable of replicating high-pressure and high-temperature engine conditions while enabling optical diagnostics for flame visualisation and data collection. In WP4, we have made significant progress in this direction with the design finalisation of our multifunctional high-temperature and high-pressure optical constant volume combustion chamber (see Figure 5.5). The chamber is currently under construction and is expected to be completed by Q4 2025.

The chamber, as shown in Figure 5.5, is specifically designed to simulate real operating conditions for reciprocating engines, with a maximum pressure capability of 12 MPa and a heating capacity up to 500 K. These specifications address key challenges in understanding ignition and flame propagation phenomena under high-pressure environments, which are crucial for optimising NH_3 combustion in engines. The spherical internal cavity ensures uniform flame propagation, while the cuboidal outer shell offers versatility in experimental configurations through modular interfaces. Each face of the shell can be equipped with specialised components, such as optical windows for high-speed imaging, pre-chamber systems for investigating flame enhancement, or gas inlet/outlet modules for precise fuel-air mixing and exhaust management. This modular design is particularly advantageous for studying diverse combustion phenomena, such as laminar flame propagation or the effect of pre-chamber geometries on combustion efficiency and stability. For instance, replacing the pre-chamber with ignition electrodes allows detailed studies of flame kernel formation and growth in premixed gases.

In parallel, we have initiated collaborative efforts with Prof Koaru MARUTA (Programme Lead, Tohoku University) to develop knock simulation models for spark-ignition NH_3 engines. These simulations aim to address critical knowledge gaps in understanding NH_3 combustion dynamics under engine-relevant conditions. The focus on knock simulations aligns closely with our overarching goal of advancing sustainable combustion systems using H_2 and NH_3.

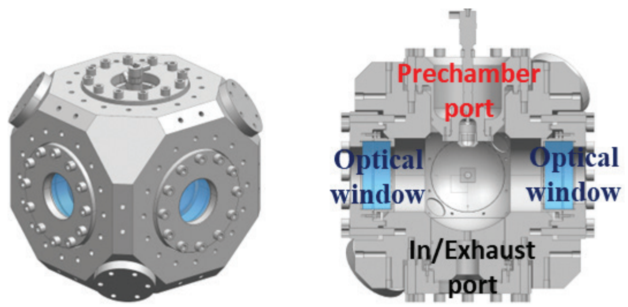


Figure 5.5: Schematic diagram of the high-pressure optical constant volume combustion chamber.

WP5: DEPLOYMENT

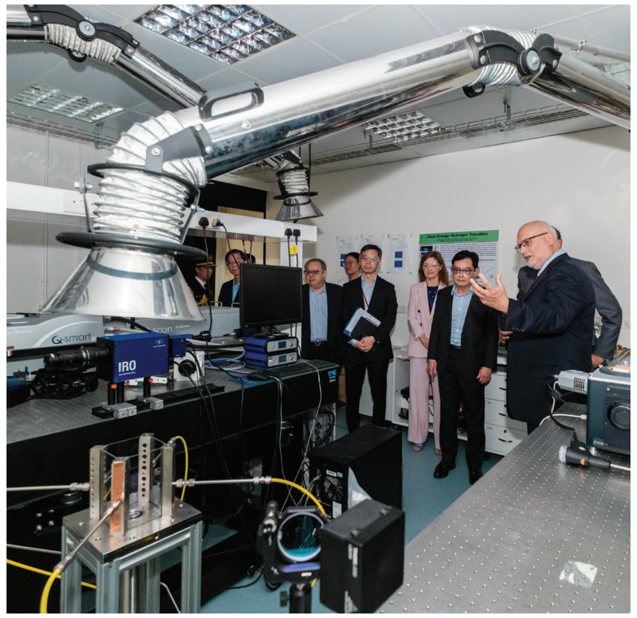
For knock prediction under NH_3/H_2 blended conditions, preliminary calculations toward a conceptual framework have commenced. These efforts focus on understanding the physical and chemical mechanisms that drive knock phenomena in alternative fuel blends. Computational Fluid Dynamics (CFD) simulations of internal combustion engine emissions have been conducted using existing setups. A parameter study on different fuel blends, including varying ratios of NH_3 and H_2, has been initiated to identify optimal conditions for minimising emissions and maximising engine efficiency. Numerical calculations are now underway to validate these findings further and refine the knock prediction framework.

For the first HYCOMBS training school, we are designing a specialised curriculum tailored for PhD students, early-stage researchers, and professional engineers. Shortlisted potential speakers from both academia and industry are currently under review. It will cover topics like combustion CFD, chemical kinetics, and gas turbine operations, with hands-on sessions using Cantera and Python for Brayton cycle calculations. We aim to hold the training program in April 2026.

OTHER ACTIVITIES AND ACHIEVEMENTS

In July 2025, Mr Tharman Shanmugaratnam, President of the Republic of Singapore, visited the CARES laboratory as part of the National Research Foundation of Singapore's presentation on the SGD$90m Decarbonisation programme which HYCOMBS is part of. Prof Epaminondas MASTORAKOS (Programme Lead, CAM) and Dr Yong Ren TAN (Research Fellow (Project Manager), CARES) showed President Tharman a flame experiment and explained the importance of the HYCOMBS research to advancing Singapore's commitment to utilising new carbon-free fuels such as hydrogen, and reaching net-zero emissions by 2050.

President Tharman (left) listening to Prof Mastorakos' introduction to HYCOMBS.



Other notable attendees at the visit were (from left to right) Mr John Lim (CEO of NRF), Prof Deborah Prentice (Vice Chancellor of the University of Cambridge), and Mr Heng Swee Keat (Chairman of NRF).

Project Leads

SM3

SUSTAINABLE MANUFACTURE OF MOLECULES AND MATERIALS IN SINGAPORE

SM3 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.

RS1 NEW SYNTHETIC STRATEGIES

We have focused on the analysis of reaction networks to establish a systematic framework for the identification of strategic “hub molecules” that act as critical intermediates, enabling the chemical transformation of “net-zero” platform molecules into target functional molecules. The “net-zero” platform molecules refer to compounds derived from sustainable raw materials such as biomass, captured carbon dioxide (CO_2), or other feedstocks that minimise reliance on fossil carbon resources. Hub molecules serve as central connectors bridging diverse reaction pathways and linking sustainable inputs to a wide array of high-value outputs. Within our project, identifying and characterising these strategic intermediates lays the foundation for streamlining synthesis planning and guiding experimental efforts towards a net-zero circular economy.

To identify strategic hub molecules, we utilised graph theory to delineate a myriad of documented chemical reactions available through open-source and commercial databases such as Reaxys, Pistachio, and Open Reaction Database (ORD). These databases compile chemical reactions reported in experimental reports, patents, and scientific journals and log various details such as reaction components (reactants, products, reagents, catalysts, and solvents), product yields, and reaction conditions. Molecular entries in the selected database were transformed into standardised forms and chemical reactions were deduplicated using robust cheminformatics protocols.

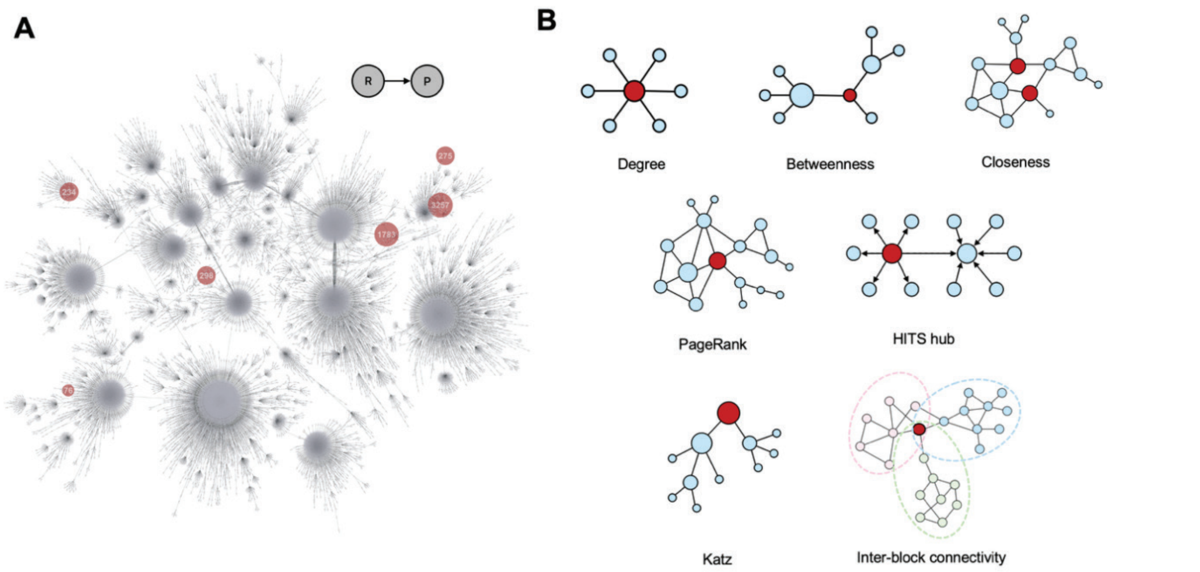


Figure 6.1: (A) A subset of a directed network graph constructed from chemical reactions obtained from Open Reaction Database (ORD). Each node represents a molecule, and each directed edge (reactant (R) to product (P)) represents reactions. The red nodes represent platform molecules such as levulinic acid, vanillin, furfural, and succinic acid. (B) Schematic representation of metrics used to enumerate nodes based on their structural influence within the reaction network. The nodes highlighted in red represent nodes with a high value for each metric.

Within this research stream, a new high-throughput synthetic facility is also being developed. Work focused on identifying key items of equipment to purchase and place orders. To date, UPLC-MS was upgraded to high-throughput mode, NMR Sample Jet was ordered, Opentrons liquid handling system was purchased and partially delivered; suppliers for high-throughput photoredox and thermal activation reaction systems were identified and orders placed. A HPLC instrument was also purchased to investigate the synthesis of aromatic ‘hub’ molecules from lignin.

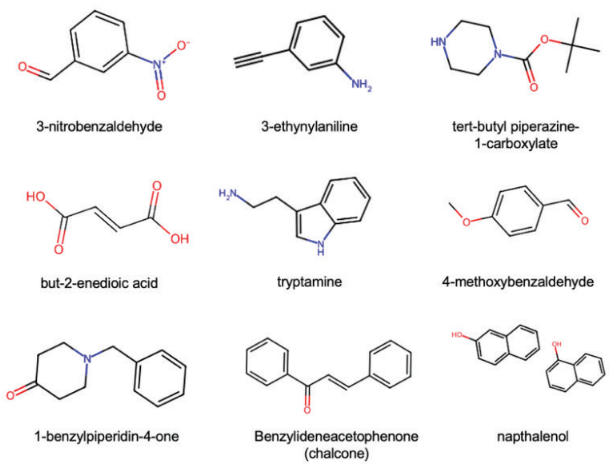


Figure 6.2: Examples of hub molecules predicted using the small-scale chemical reaction network constructed using reaction dataset extracted from ORD.

RS3 SCALABILITY OF SYNTHESIS TECHNOLOGIES

The work on technology mapping aims to develop a library of process models that cover most common technologies in pharma manufacturing, including novel synthesis technologies, such as sonochemistry, light-activation and light-current activation. We are building models using a modular approach, such that underlying models could be re-used in multiple use scenarios. The models are developed on an established semantic knowledge graph ontology that captures variables, laws, phenomena, rules and process context for bottom-up/top-down assembly of mechanistic models and subsequently an object-oriented modular simulation environment that enables plug-and-play integration of unit operations and dynamic plant-scale studies.

Several first principles models for key unit operations are documented, built and implemented from literature sources, see Table 1. Notably, two required dynamic unit operations models were assembled in the simulation environment; a dead-end membrane filter press, with Darcy-based flux, cake growth, cleaning logic and energy inventory calculations, along with a slightly simplified model of a jacketed batch crystallizer, simulating overall-rate supersaturation kinetics, reactor and jacket energy balances and utility consumption tracking, omitting Particle Size Distribution (PSD). Additionally, a surrogate mechanochemistry ball mill reactor model was formulated within the knowledge of the ontology for the SM_3 case study, representing impact energy, collision frequency and first-order conversion parameterised by specific energy input.

Table 1. Status of models development for the first part of SM_3 case studies and required unit operations for the simulation environment.

Unit operation	Ontology	Simulation environment
Ball mill	Simplified model (PBM under development; comparison planned)	Planned
Sonochemistry	Planned	Planned
Crystallization	N/A	Completed (batch, jacketed, no PSD)
Membrane filter press	N/A	Completed (dead-end)
Distillation	N/A	In progress (batch flash)

RS4 SUSTAINABILITY, SYSTEMS AND ARTIFICIAL INTELLIGENCE

The work on process chain design and techno-economics focuses on developing methods for technoeconomic analysis (TEA) of the novel synthesis technologies and the proposed technologies for manufacture of net-zero molecules. The automation of TEA for new technologies demands the creation of a framework that reduces the amount of guesswork needed to perform and compare TEA studies by incorporating data-driven and modular approaches within a clearly defined scope. The first phase of building such a software involves the implementation of methods from chemical engineering textbooks; these are primarily based on old data but are still widely utilised in academia because of the lack of access to proprietary cost data. The equipment cost equations are first extracted from the textbooks and compiled into SQL databases. The types of equipment included in the database are shown in Table 2.

Table 2. Compilation of equipment classes with cost equations obtained from textbooks.

Liquid reactor	Particle size control	Distributor	Other separator
Gas reactor	Heat exchanger	Agitator	Membrane
Storage tank	Power and driver	Crystalliser	Solid handling
Power generation	Vessel	Solid-liquid separator	Mixer for solids
Turbomachinery	Trays and packing	Solid-gas separator	Vacuum system

The cost models derived from these methods can then be systematically compared with commercial software such as Aspen Process Economics Analyzer (APEA) to determine where differences occur. For example, Figure 6.3 shows a comparison between the purchased and installed costs, obtained using different methods, of a simple stirred tank reactor and a U-tube shell-and-tube heat exchanger. The method resulted in an estimated purchased cost of the reactor that was twice that of the value from APEA, while the online equipment cost calculator, produced a closer estimate. More notably, the textbook estimated installed cost was more than three times that from APEA, highlighting a potential weakness of the method and warranting further investigation.

These cost models can potentially be calibrated against commercial software, new cost data, and even expert opinion to produce estimates that are more reliable and comparable as opposed to those obtained from individual methods arbitrarily selected by researchers. Provisions for scenario and uncertainty analyses will also be added subsequently, which can aid decision making when accounting for potential policy changes and market fluctuations.

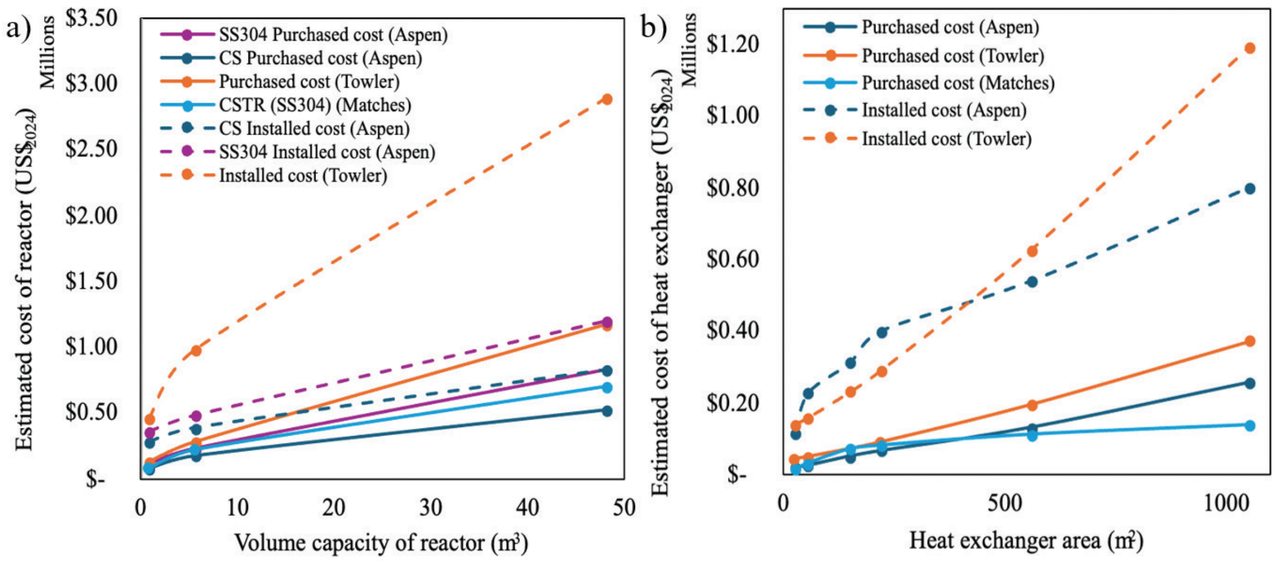
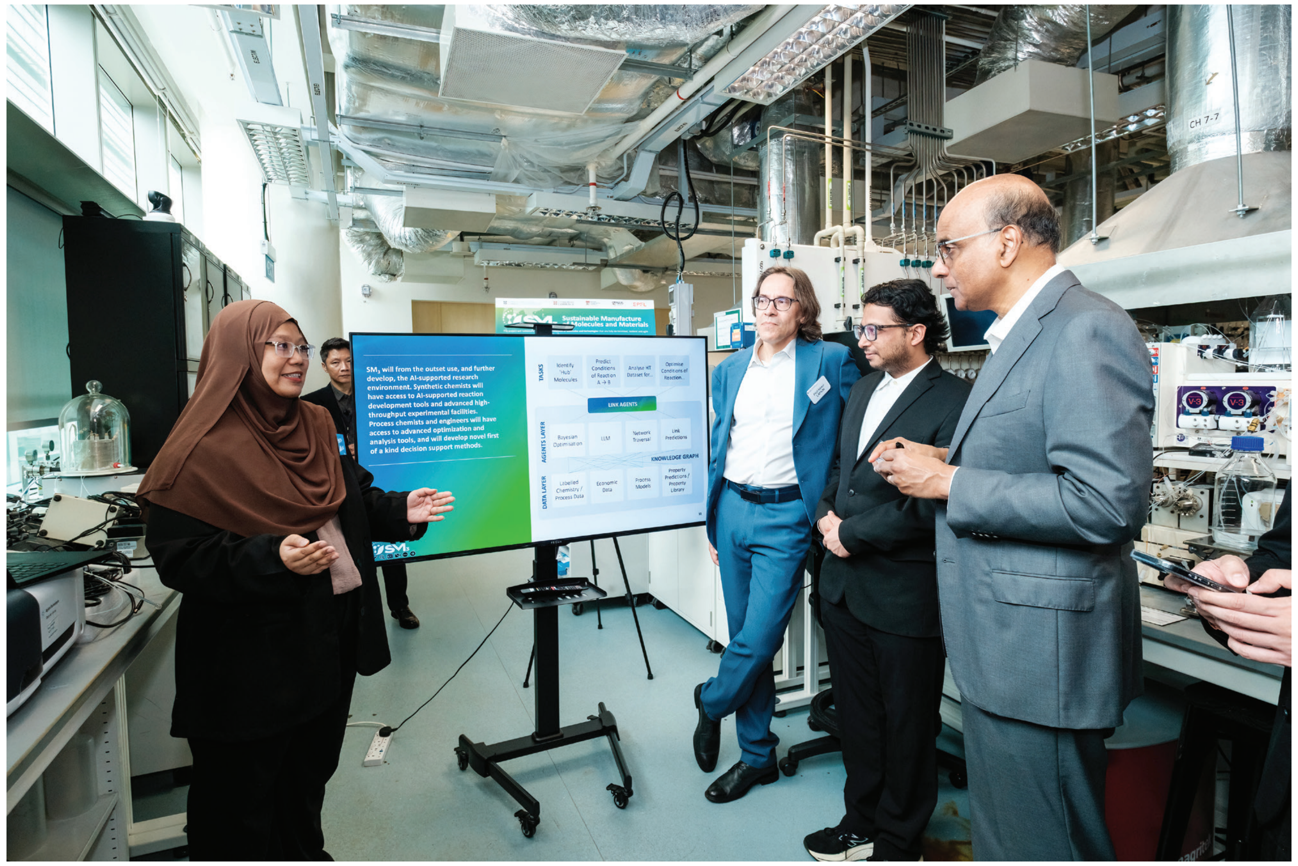


Figure 6.3: Comparison of the purchased and installed costs estimated from Aspen Plus, and the equipment cost calculating website Matches, for (a) a continuous stirred tank reactor and (b) a U-tube shell-and-tube heat exchanger.

OTHER ACTIVITIES AND ACHIEVEMENTS

In July 2025, Mr Tharman Shanmugaratnam, President of the Republic of Singapore, visited the CARES laboratory as part of the National Research Foundation of Singapore's presentation on the SGD$90m Decarbonisation programme which SM_3 is part of. Prof Alexei LAPKIN (Programme Lead, CAM), Asst Prof Tej CHOKSI (PI, NTU), and Dr Raudah LAZIM (Research Fellow, CARES) explained the importance of SM_3 in looking for alternative non-fossil fuel sources in the chemical industry supply chain, leveraging Singapore's position as a hub for chemical manufacturing and trade to collaborate with industry.

Additionally, CARES and the University of Cambridge have signed a contract through which Chemical Data Intelligence (CDI) Pte Ltd has committed to co-fund a PhD student within the SM_3 project. Furthermore, CDI has fully funded a PhD student at the University of Cambridge to work on an additional research question, relating to scalability of novel synthesis technologies.



President Tharman (right) listening to Dr Raudah Lazim's introduction to SM_3. Pictured also are Prof Alexei Lapkin and Asst Prof Tej Choksi.

HD4

HEALTH-DRIVEN DESIGN FOR CITIES

HD4 is a groundbreaking collaboration that brings together world-class researchers from Nanyang Technological University, National University of Singapore, and the University of Cambridge. HD4 will investigate how individuals live and move in Singapore, how the urban environment shapes their exposure to health risks, and how this influences their behaviour and health.

People living in cities face growing challenges to their health and wellbeing: heat, noise, air pollution, and limited opportunities to eat healthily and be physically active.

HD$_4$ is integrating environmental data with health and behaviour data in 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. As a city with ambitious health goals, rich data, and the drive to turn research into real change, Singapore offers a unique setting. HD$_4$ will work in partnership with government agencies, so that the science can guide Singapore's planning and health strategies in the years ahead.

Professor John Chambers
HD4 Programme Lead, NTU

Professor Nick Wareham
HD4 Programme Lead, CAMBRIDGE

Research Objectives

HD$_4$ will undertake research in the following areas:

- Characterising features of the Singapore environment that potentially impact health
- Understanding the links between environmental factors, individual behaviour and health outcomes
- Observing the impact of environmental change on health in Singapore
- Working with government agencies to explore the development of useful public health tools.

Research Team

The HD$_4$ team has been busy recruiting and we are expecting to have filled all positions imminently. We were joined by existing researchers Dr Theresia MINA, Dr Wubin XIE, Dr Dorrain LOW, Dr Xiaoyan WANG and Dr Akash BAHAI at NTU, and welcomed new researchers Dr Jielin CHEN, Sharyl CHIN, and Dr Thi Ang Hong NGUYEN at CARES.

Programme Lead Prof Nick WAREHAM, Deputy Programme Lead Prof Ronita BARDHAN, investigators Prof James WOODCOCK, Dr Louise FOLEY, Dr Søren BRAGE and Dr Tom BURGOINE, Oliver FRANCIS (Specialist Collaborator) and Dr Jethro AKROYD (Scientific Programme Manager) were resident at CARES over the summer, contributing to the inaugural HD$_4$ Summer Seminar Series. The time spent in Singapore was valuable, building team cohesion and moving the research forward at pace.

Research Plan

HD$_4$ will proceed in two phases. The critical contribution of the current phase of HD$_4$ – Phase 1 – is to test feasibility and deliver proof-of-concept analyses to establish a foundation for subsequent research. This will pave the way for Phase 2, which will identify interventions to help improve the health of Singaporeans.

Project Leads


Professor Nick WAREHAM
University of Cambridge


Professor John CHAMBERS
Nanyang Technological University


Assoc Professor
Rudi STOUFFS
National University of Singapore


Professor Ronita BARDHAN
University of Cambridge

SCIENTIFIC UPDATES

Urban environmental exposures for SG100K participants

Leads

Prof Ronita BARDHAN (CAM)
Assoc Prof Rudi STOUFFS (NUS)

HD_4 has developed a framework to identify the most relevant urban environmental exposures that may affect health and mapped out how these can be measured. Alongside this, a data pipeline has been created to link information on individual point-based environmental exposures with SG100K data. This system has been tested using preliminary green space data.

The team is designing methods to capture a richer picture of green space. These include measuring accessibility and inclusivity, distinguishing between formal and informal green spaces, and assessing the diversity of greenery across neighbourhoods. Automated techniques are also being developed to analyse satellite imagery, allowing calculation of long-term indicators such as vegetation cover, surface temperature, and water presence.

Work is progressing on new ways to measure heat and humidity exposure. A climate index is being developed using a combination of physical modelling and deep-learning weather predictions. To support this, high-resolution models of building and canopy heights have been generated, enabling more precise calculations of sky view factor (the openness of the sky above).

In parallel, the team has begun using OpenStreetMap data to model walking and cycling networks in Clementi, providing a proof-of-concept for accessibility-based exposure metrics. A manuscript has been submitted demonstrating how GPS data can be used to calculate dynamic exposures over time, taking into account both historical and current features of the environment. This work, drawing on projects in both Singapore and the UK, shows how the methods can be applied internationally.

Figure 7.1: Point-based green space exposure metrics showing the difference before and after the Gallop extension of the Botanical Gardens for 400, 800 and 1,000 m buffer sizes.

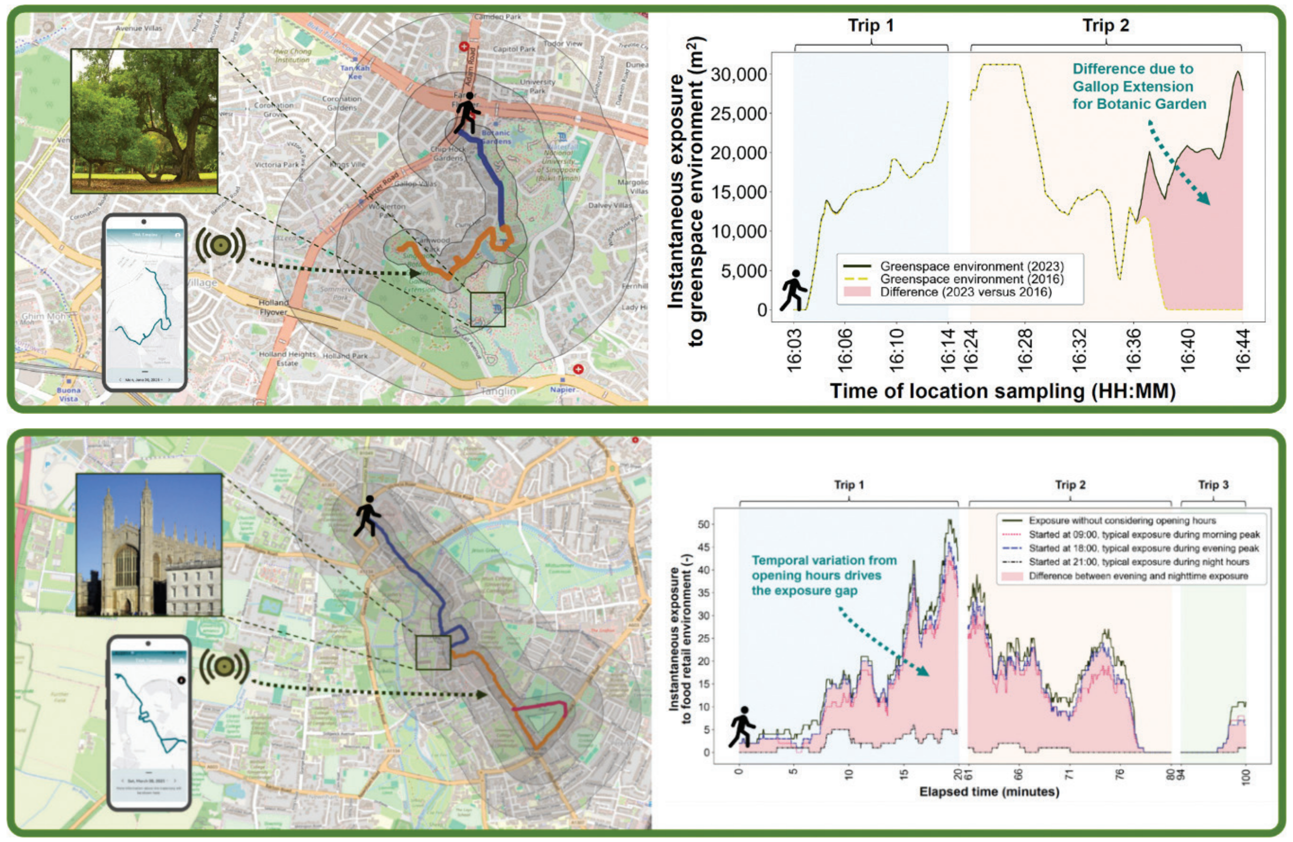


Figure 7.2: Proof-of-concept for using GPS data to estimate environmental exposures to green space in Singapore (top) and food retail in Cambridge (bottom).

Relationship between environments and health-related behaviours

Leads

Asst Prof Marie LOH Chiew Shia (NTU)
Dr Louise FOLEY (CAM)
Dr Jenna PANTER (CAM)

A preliminary analysis to explore the link between green space exposure and self-reported physical activity was used to test the new data pipeline. A detailed analysis plan is now being developed to study the relationship between environmental factors, and self-reported and objectively measured physical activity in Singapore.

Key health behaviours have been characterised using data from the first 10,000 participants in SG100K. This group provides the most comprehensive data to date, covering behavioural, clinical, and molecular measures. These analyses lay the foundation for further work across the full cohort, enabling comparisons across different sociodemographic groups and geographic areas, and incorporating more objective lifestyle measures.

Other studies are underway to examine sleep and adiposity, revealing important ethnicity-related differences in sleep quality. Dietary data are being expanded to include internationally recognised indices and dietary patterns. In parallel, collaborative student projects between NTU and Cambridge have contributed to analyses of ultra-processed food intake and protein consumption. Cardiorespiratory fitness has been characterised and its associations with metabolic health investigated to enrich physical activity traits. Collectively, these developments are strengthening the lifestyle measures that can be applied to the full SG100K dataset.

Relationship between environments, behaviours, and health

Leads

Prof John CHAMBERS (NTU)
Assoc Prof Xueling SIM (NUS)
Prof Nita FOROUHI (CAM)

The SG100K Health Informatics team, led by Senior Research Fellow Dr Theresia MINA, has built strong foundations for linking environmental, behavioural, and health data. Their work ensures data are carefully quality-controlled, versioned, and documented, and that health records can be securely connected to other datasets.

A structured dictionary of environmental variables has been developed, allowing environmental exposures to be linked to individual health data. A preliminary analysis of the first 10,000 participants revealed negative associations between green space exposure and cardiometabolic risk factors. Further studies are in progress, exploring links between health outcomes and exposures such as physical activity, adiposity, diet, and fitness. A perspective paper on adversity, diet, and health in Asian populations is in preparation.

The team is building a statistical pipeline to generate lifestyle variables at scale for the entire SG100K cohort. In addition, they are implementing the analysis pipeline used in the UK Biobank to process physical activity data for more than 25,000 participants using NTU's high-performance computing facilities.

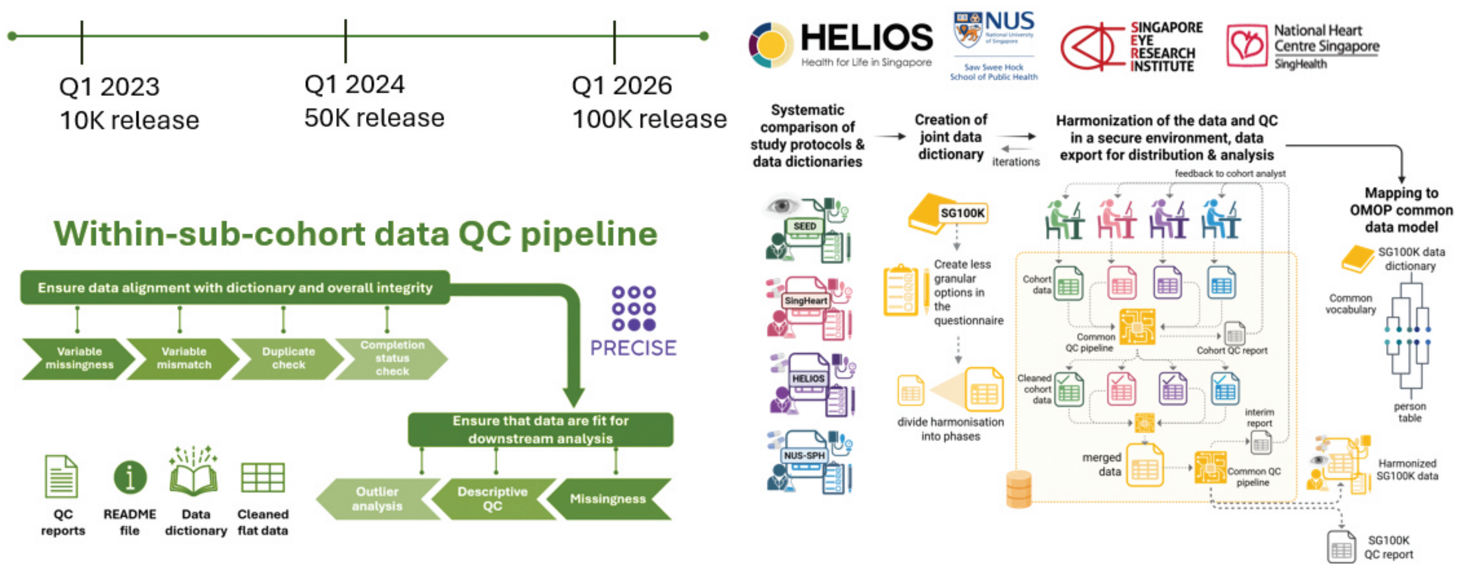


Figure 7.3: General data pipeline to generate lifestyle phenotype and health outcomes.

Novel approaches for improving assessment of person-level environmental and behavioural exposures

Leads

Dr Søren BRAGE (CAM)
Assoc Prof Falk MÜLLER-RIEMENSCHNEIDER (NUS)
Assoc Prof Jason Kai Wei LEE (NUS)

Work is underway to test methods for SG100K to measure health and lifestyle remotely. This feasibility study will involve 200 participants drawn from the wider cohort and will help establish practical, scalable approaches for future large-scale assessments.

Participant recruitment is being carefully planned. Instead of relying solely on remote invitations, which often lead to low response rates, participants attending their baseline clinical assessments will be invited to take part in this digital add-on study. This integrated approach will ensure efficiency while providing participants with an additional opportunity to contribute to research.

Several areas of remote data collection are being explored:

- **Location and movement tracking:** Secure data flows have been established to enable GPS and physical activity monitoring through both iOS and Android smartphones. While phone-based heart rate monitoring has proven unreliable across different devices, Singapore's national Healthy 365 programme offers wrist-worn activity trackers, which provide a promising alternative. Discussions are ongoing to access this platform for research purposes.
- **Dietary assessment:** The remote study will use a Singapore-specific version of the Intake-24 dietary recall tool. In parallel, we are exploring the possibility of using the new diet-tracking features, including meal photo capture, that are available via Healthy 365.
- **Indoor environment monitoring:** Different sensors are being tested to measure indoor air quality. Preliminary comparative data have been collected, and work is ongoing to develop secure systems for transferring these measurements to the research team.

The next step will be to finalise the technical solutions before submitting an ethics application. Recruitment of participants will begin once approval is granted.

Dr Søren BRAGE (left) and Yuan WANG (right).

Making an impact through engagement

Leads

Dr Thomas BURGOINE (CAM)
Dr Yih Yng NG (NTU/NUS)
Asst Prof Bernett LEE (NTU)
Assisted by Specialist Collaborator Oliver FRANCIS (CAM)

We are delighted to welcome Sharyl CHIN as Knowledge Broker for HD_4. Based at CREATE Tower on the NUS campus, Sharyl plays a central role in connecting research with policy and practice.

HD_4 works closely with government agencies to share knowledge and co-create research with real-world impact. A key initiative is the **Stakeholder Advisory Group**, which provides an open channel for two-way communication with agency partners. The group held its first meeting in August 2025 at CREATE Tower, bringing together representatives from the Urban Redevelopment Authority (URA), Housing Development Board (HDB), Health Promotion Board (HPB), MOH Office for Healthcare Transformation (MOHT), Ministry of National Development Centre for Liveable Cities (MND CLC), National Environment Agency (NEA), NParks, Public Sector Science & Technology Policy and Plans Office (S&TPPO), and the Singapore Land Authority (SLA).

The Stakeholder Advisory Group meeting was lively and informative, offering valuable perspectives that will guide our research in the months ahead. The group will reconvene every six months, with ongoing engagement between HD_4 staff and agency colleagues to ensure continuous collaboration. Plans are also underway for a visit to URA headquarters, including a guided tour of the Singapore City Museum. These activities are designed to strengthen dialogue and foster a shared understanding of Singapore's public health challenges and potential solutions.

Alongside stakeholder engagement, HD_4 is communicating its research more widely through traditional media, social media, newsletters, and via dedicated website. This year saw the launch of the **HD_4 brand identity** – including a new logo, colour palette, and fonts – that has already been applied across our communications. Highlights include the redesigned HD_4 website, a growing presence on LinkedIn, and a **printed HD_4 introduction brief** distributed to partners and collaborators.

The new branding was unveiled at the inaugural HD_4 Summer Seminar Series, which featured in-person lectures from HD_4 investigators and partners in Singapore. Beyond academia, HD_4 representatives also met with Science Centre Singapore to explore opportunities for public outreach. These efforts mark an important step in ensuring that HD_4's work resonates across both policy and community settings.

HD_4 introduction brief distributed to partners and collaborators.

Attendees at the final event in the HD_4 Summer Seminar Series, 25 August 2025.

CONFERENCE PRESENTATIONS

Assoc Prof Rudi STOUFFS and researcher Yuan WANG presented work relating to HD4 at international conferences.

- *"Impacts of Building Height and Local Climate Zones on the Performance of the InVEST Urban Cooling Model"* was accepted as a full paper and delivered as an oral presentation at the SBE25 Conference in Zurich from 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"* was delivered as an oral presentation at the 12th International Conference on Urban Climate (ICUC 12) in Rotterdam from 7 - 11 July 2025.

Closer to home, researchers Dr Jielin CHEN, Dr Wubin XIE, Dr Theresia MINA, Dr Mutian MA and Sharyl CHIN have submitted an abstract to the Singapore Science Conference 2025 on behalf of the HD_4 programme.

Find out more: www.cares.cam.ac.uk/research/hd4-project

Contact: HD_4 Knowledge Broker Sharyl Chin, sharyl.chin@cares.cam.ac.uk

AMPLE

AN ACCELERATED MANUFACTURING PLATFORM FOR ENGINEERED NANOMATERIALS

Accelerated Materials 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
University of Cambridge

SCIENTIFIC UPDATES

Trials at Elite Advanced Materials on the K100 system have been completed successfully, with a successful demonstration of continuous operation over a day. Dr Nicholas JOSE (Project Lead, CARES) can be seen with the system in the picture below. Significant improvements have been made to stabilise the system in the reactor design, setup and automation, led by Mr Thiru SELVARAJ (Chemical Process Technician, CARES). Digital twinning software has been incorporated using the digital twin developed in collaboration with the Pharma Innovation Programme Singapore (PIPS) via Dr Mohammed JERAAL (Materials Engineer, CARES) to include additional automated controls and interlocks. This work will be presented at AICHE 2025 in Boston, USA.

PUBLIC ENGAGEMENT

The AMPLE team has engaged with the public to present the achievements of the project and the resulting spin-off, Accelerated Materials, through a number of events:

- Dr Jeraal presented, "Building Self-Driving Laboratories: A Practical Introduction for Experimental Researchers" at the 8th Machine Learning in Biotechnology and Chemical Engineering conference in Cambridge, UK from 1 - 2 July 2025.
- Dr Jeraal presented, "Building Self-Driving Laboratories: A Practical Introduction for Experimental Researchers" at the inaugural AI4X conference in Singapore from 8 – 11 July 2025.
- Dr Jeraal presented "Revolutionizing Materials Discovery and Manufacture" at the NAMIC Startup Innovation Forum in Singapore on 15 September 2025.
- Accelerated Materials displayed an exhibition booth at ACHEMA Asia in Shanghai from 14 – 16 October 2025. Dr Mikhail KOVALEV (Technical Development Manager, CARES) attended with other AM staff members, Mr Kelvin YEO and Ms Kylie CHUA, who were successfully converted from AMPLE to AM following the company's successful seed round campaign.
- Dr Jeraal has been invited as a speaker in the upcoming Singapore Week of Innovation & Technology (SWITCH) Beyond event, a deep tech track that delivers intensive, domain-focused sessions for participants seeking to understand and shape the future of deep tech. He will be speaking for the track "AI for Materials" on 30 October 2025.
- The Accelerated Materials journey was also documented by the company's CEO, Dr Nicholas JOSE; and CSO, Prof Alexei LAPKIN, in Nature Chemical Engineering's first Down to Business article, titled "A roadmap toward closed-loop autonomous experimentation for engineered nanomaterials". (DOI: 10.1038/s44286-025-00291-x)

PUBLICATIONS

A Roadmap toward Closed-Loop Autonomous Experimentation for Engineered Nanomaterials

Jose, N. A.; Lapkin, A. A., *Nature Chemical Engineering*

https://doi.org/10.1038/s44286-025-00291-x

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.

Project Leads


Professor Alexei LAPKIN
University of Cambridge


Dr Ann CHOW
A*STAR


Professor Mick MANTLE
University of Cambridge


Prof Dame Lynn GLADDEN
University of Cambridge

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.

SCIENTIFIC UPDATES

Automated evaluation of environmental impacts of pharma manufacturing processes

The three-year project that started in July 2023 is 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.

In recent months the project focused on developing the standard technology for maintaining process models and calculations of process flowsheets. This technology is the backbone of our approach to generate accurate estimates of life cycle inventories. This work is done in close collaboration with Chemical Data Intelligence (CDI) Pte Ltd.

Dr Dogancan KARAN (Research Fellow, CARES) has completed the model libraries for waste water processes with the data gathered from 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/simulation environment which consists of different unit operations, mathematical models and high-level functions to orchestrate the entire process flow sheet and run simulations. An example of process flow sheet creation and estimation of the carbon footprint for a wastewater treatment process is demonstrated in Figure 8.1. This flowsheet is simulated for a treatment of a biological waste mixture with V = 45 m^3, T = 35 °C and pH = 2. Simulation environment runs the process and estimates the life cycle inventory of the process. From the life cycle inventory and the impact factors of different utilities, the carbon footprint of the process is estimated to be 0.55 kg CO_2 equivalence per 1m^3 waste. In the next 6 months, Dr Karan will be working on expanding the model libraries for upstream processes and thermodynamic calculations.

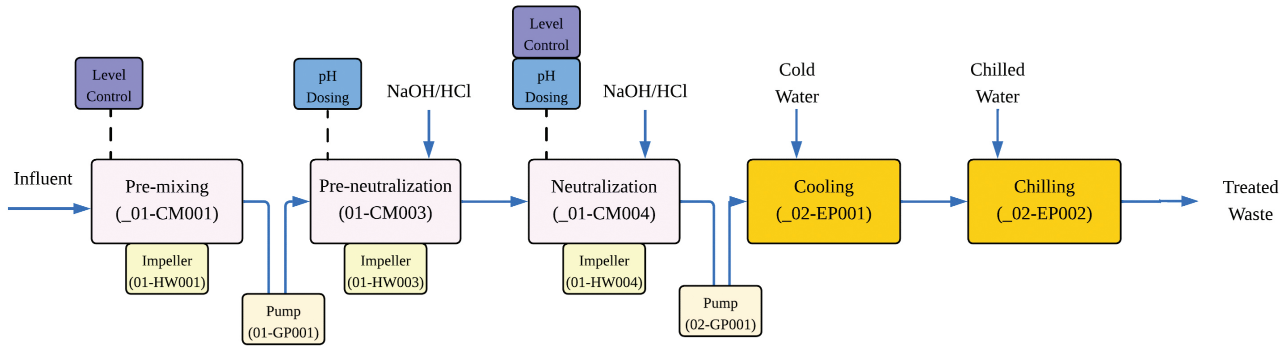


Figure 8.1: Schematic representation of a flowsheet created by model libraries and simulation environment.

Building a Capability in Magnetic Resonance Methods for the Pharmaceutical and Agrochemical Sector within PIPS

The PIPS project commenced in July 2025 led by Dr Ann CHOW (A*STAR), Prof Mick MANTLE (CAM), and Prof Dame Lynn GLADDEN (CAM). Since then, recruitment for the Postdoctoral Research Associate (PDRA) position has commenced. At the time of writing, interviews have been conducted, and the recruitment process is ongoing. A final decision and appointment is expected in mid-November.

The project is divided into five work packages (WPs). Their overarching aim is to use magnetic resonance imaging, relaxation/diffusion, and spectroscopic methods to better understand how the operating conditions of heterogeneous hydrogenation reactions, carried out in continuous-flow microscale trickle-bed catalytic reactors, can be optimised to improve reactor performance in terms of conversion and selectivity.

Contact has been established between Cambridge and industrial partners regarding the catalysts currently used in industry. These spherical, carbon-based catalyst supports have been sent to Cambridge. Preliminary screening experiments were performed to ensure that the radio-frequency (r.f.) coils used in magnetic resonance experiments are not adversely affected by the carbon-based materials.

Other activities have included the transfer of model T_1–T_2 and D–T_2 magnetic resonance datasets to the A*STAR Magnetic Resonance Group, led by Dr Chow, to address potential hardware and data-processing software compatibility issues.

In October, Cambridge carried out initial testing of T_1–T_2 and D–T_2 pulse sequences on their 400 MHz magnetic resonance spectrometer using a sample of one of the carbon-based catalyst supports imbibed with methanol, a typical solvent used in the heterogeneous catalytic hydrogenation reactions of interest to industrial partners. Figure 8.2 shows the results of a two-dimensional T_1–T_2 relaxation correlation experiment, which provides insight into how methanol interacts with the surfaces of the porous carbon support.

Once the PDRA has been appointed, the initial work will focus on Work Packages I and II, which aim to: (I) use magnetic resonance imaging to visualise fluid flow behavior and provide insight into regions of hold-up, turbulence, backflow, fast flow, and stagnation in a model microscale trickle-bed reactor (TBR); and (II) continue the T_1–T_2 and D–T_2 pulse sequence development and optimisation for carbon based catalyst supports.

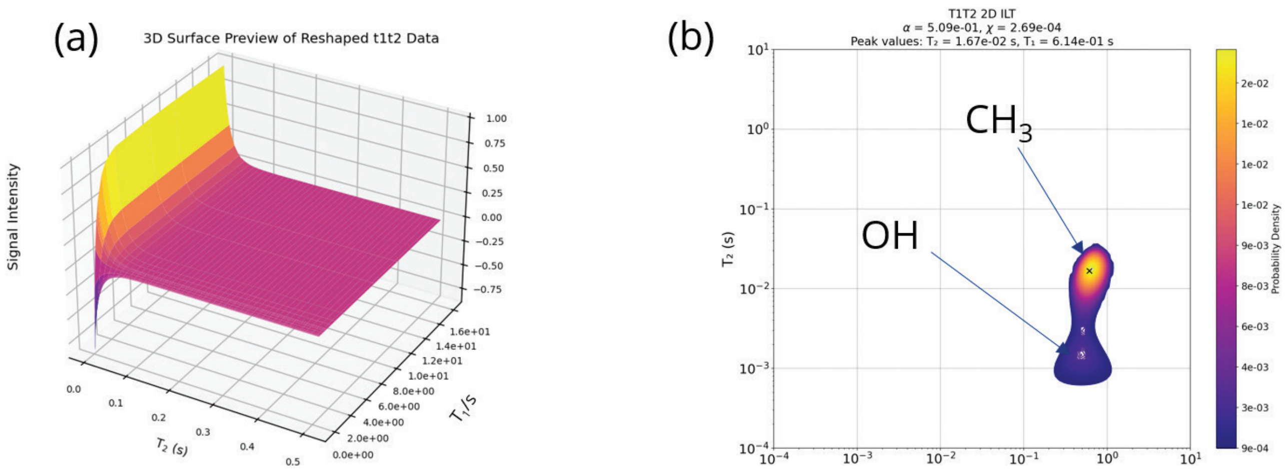
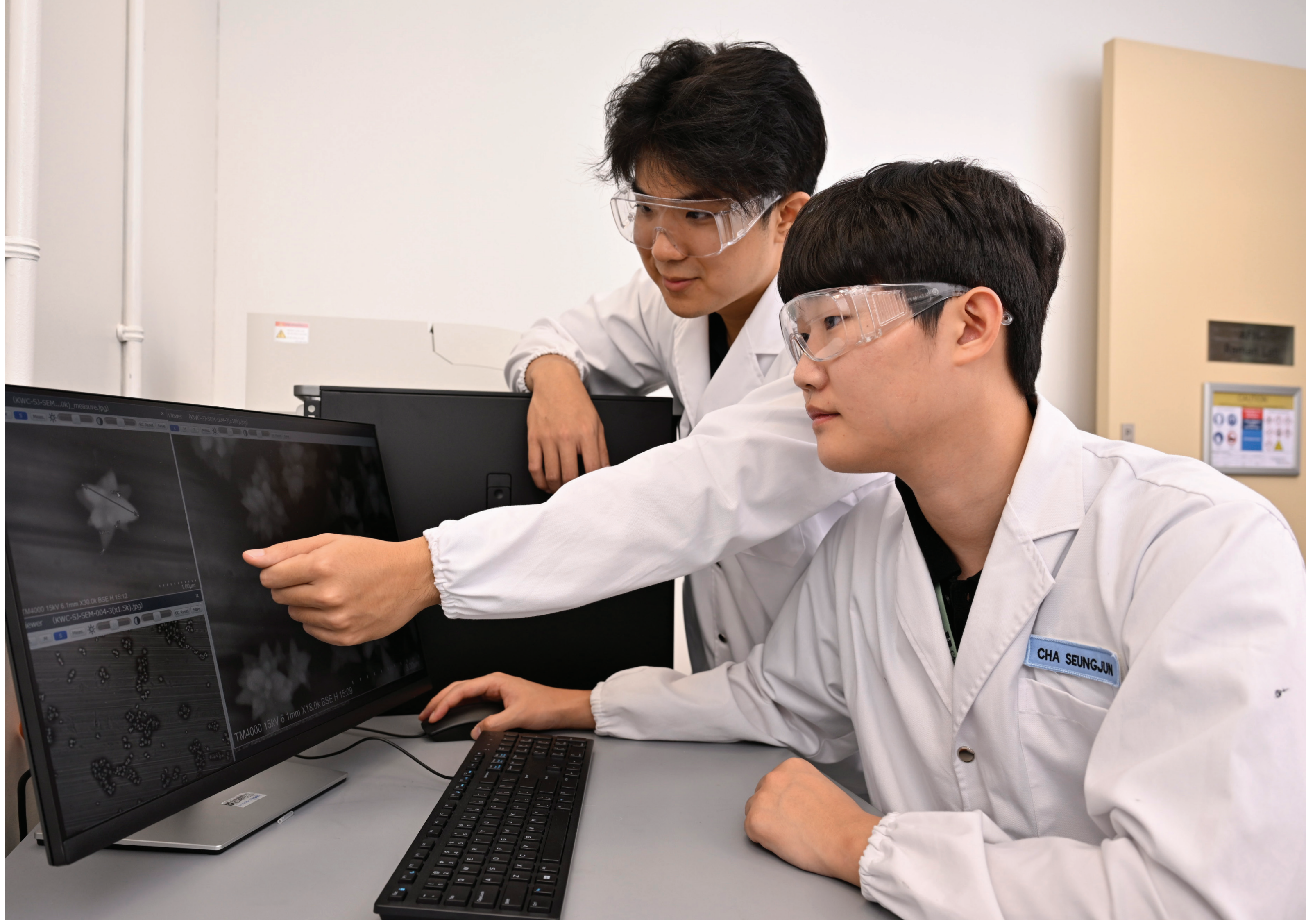


Figure 8.2: (a) Raw T1-T2 time domain magnetic resonance data shown as a 3D surface plot for methanol imbibed in a carbon-based catalyst support. (b) The 2D numerical inversion of (a) highlighting the two chemical species present in methanol and indicating (via a lower T2 value) the stronger interaction of the OH group of methanol with the surface of the carbon based support.

OTHER ACTIVITIES AND ACHIEVEMENTS

An earlier PIPS project, PIPS DF2 From Digital Twins to Real Time AI-supported Plant Operation, closed in July 2025. A press release was issued by CARES in conjunction with a project summary video that is available for public viewing.

Prof Alexei LAPKIN (PI, CAM) was invited for a follow-up interview with PharmaManufacturing.com, "University of Cambridge research arm develops AI digital twin for pharma manufacturing".



Other Projects

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, hire interns (pictured above), or build relationships with new industry partners and 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.

LOW-CARBON ENERGY RESEARCH PHASE 2

In collaboration with the National University of Singapore

Dr B. HARIKRISHNAN (Research Fellow, CARES) has been contributing to the **LCER** project, which focuses on developing and applying the Incompletely Stirred Reactor Network (ISRN), a low-order modelling approach designed for computationally efficient and rapid parametric analysis of NOx emissions. The ISRN acts as a post-processing tool that leverages mixing fields from high-fidelity LES simulations, particularly LES-CMC (Large Eddy Simulation with Conditional Moment Closure).

The high-fidelity **LES-CMC** simulations were conducted based on the experimental conditions of the SINTEF sequential combustor operating with cracked ammonia fuel (Ditaranto and Saanum, 2024). **Anchor-point** simulations were performed for selected decomposition ratios (DR), followed by ISRN analyses to predict NOx emissions under 10 bar pressure and a primary zone equivalence ratio (ϕ_{pz}) of 1.5. Multiple chemical mechanisms were employed and compared in the ISRN framework to assess predictive consistency.

Additional simulations were conducted for DRs of 0.5 and 0.9 at 5 bar pressure, ϕ_{pz} of 1.0, and 50.2 kW power. The corresponding mixing fields will be extracted and used to further validate the low-order ISRN predictions, which forms the next objective of the study.

The next phase of the research will extend the application of these emission prediction techniques to an industrial burner from **SIEMENS Energy**, aiming to demonstrate the model's capability under practical operating conditions.

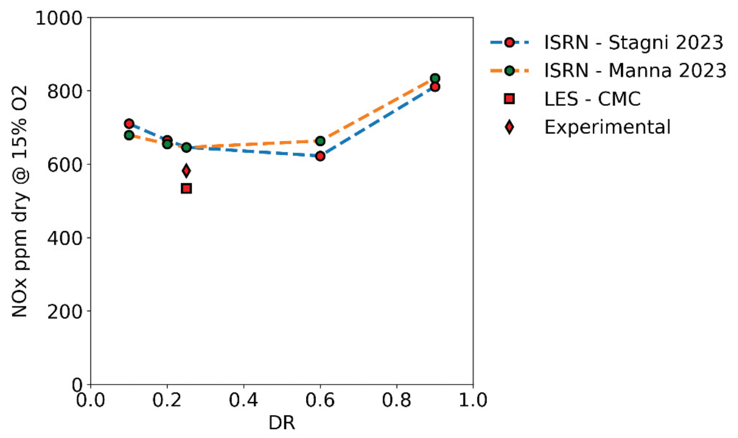


Figure 9.1: Comparison of NOx emissions for different chemical mechanisms for the cases with pressure 10 bar and primary zone equivalence ratio (ϕ_{pz}) 1.5.

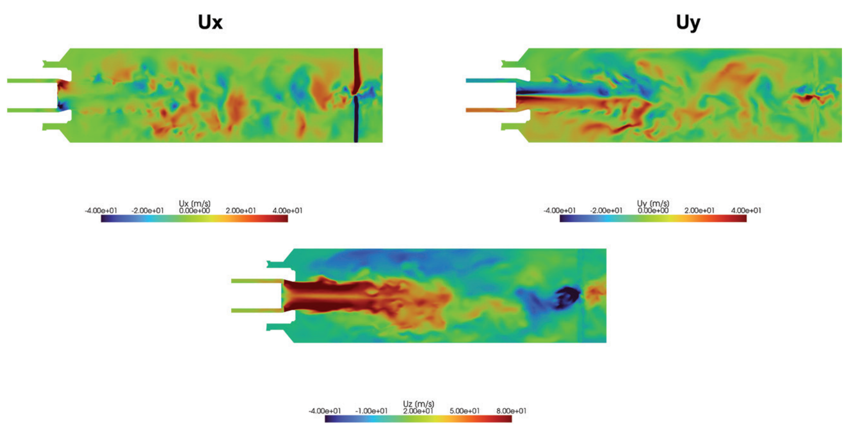


Figure 9.2: Velocity fields for the anchor point LES-CMC simulation with decomposition ratio (DR) 0.5, primary zone equivalence ratio (ϕ_{pz}) 1.0, and power 50.2 kW.

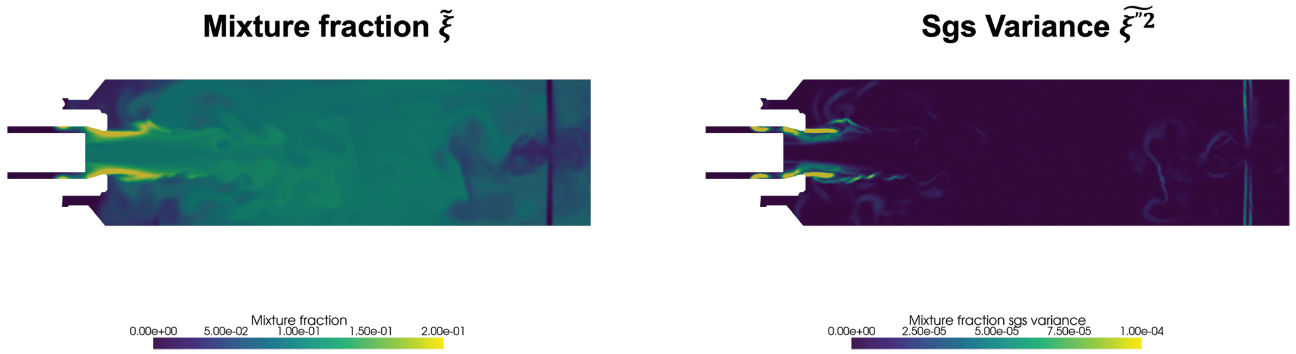


Figure 9.3: Mixing field statistics for the anchor point LES-CMC simulation with decomposition ratio (DR) 0.5, primary zone equivalence ratio (ϕ_{pz}) 1.0, and power 50.2 kW.

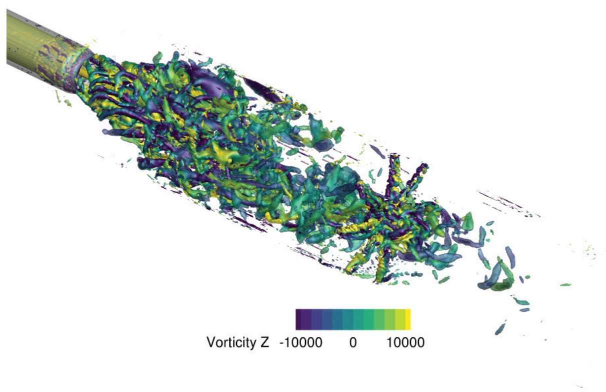


Figure 9.4: Iso-surfaces of Q-criterion for the anchor point LES-CMC simulation with decomposition ratio (DR) 0.5, primary zone equivalence ratio (ϕ_{pz}) 1.0, and power 50.2 kW. The iso-surfaces are coloured by the z- vorticity.

References

Ditaranto, M.; Saanum, I. Experimental Study on the Effect of Pressure on Single and Two Stage Combustion of Decomposed Ammonia (NH3 H2 N2) Blends over a Swirl Stabilized Burner. *Combustion and Flame* 2024, 262, **113368**. https://doi.org/10.1016/j.combustflame.2024.113368.

OTHER ACTIVITIES AND ACHIEVEMENTS

Dr B. HARIKRISHNAN (Research Fellow, CARES) presented part of his work in a paper titled "Predictive modelling of ammonia combustion systems: Coupled LES-CMC and ISRN approach" at the 11th International Symposium on Turbulence, Heat and Mass Transfer from 21 – 25 July 2025 in Tokyo, Japan.

Dr Harikrishnan will be presenting another part of his work at the upcoming 22nd International Conference on Flow Dynamics in Sendai, Japan.

PUBLICATIONS

Publications

ALL PUBLICATIONS WITH CREATE ACKNOWLEDGEMENT

Newly added publications for this reporting period are coloured in red. For a full record of earlier publications, please visit our Publications page on the CARES website

C4T impact-focused "CN" projects

Ayachi, F.; Law, L. C.; Mastorakos, E.; Romagnoli, A. Comparative Techno-Economic Analysis of Integrated Process Designs Combining LNG Cold Utilization and Carbon Capture. *Journal of Cleaner Production* 2025, *524*, 146274. https://doi.org/10.1016/j.jclepro.2025.146274.

Bai, J.; Lee, K. F.; Hofmeister, M.; Mosbach, S.; Akroyd, J.; Kraft, M. A Derived Information Framework for a Dynamic Knowledge Graph and Its Application to Smart Cities. *Future Generation Computer Systems* 2024, *152*, 112–126. https://doi.org/10.1016/j.future.2023.10.008.

Bai, J.; Mosbach, S.; Taylor, C. J.; Karan, D.; Lee, K. F.; Rihm, S. D.; Akroyd, J.; Lapkin, A. A.; Kraft, M. A Dynamic Knowledge Graph Approach to Distributed Self-Driving Laboratories. *Nat Commun* 2024, *15* (1), 462. https://doi.org/10.1038/s41467-023-44599-9.

Bai, J.; Rihm, S. D.; Kondinski, A.; Saluz, F.; Deng, X.; Brownbridge, G.; Mosbach, S.; Akroyd, J.; Kraft, M. Twa: The World Avatar Python Package for Dynamic Knowledge Graphs and Its Application in Reticular Chemistry. *Digital Discovery* 2025, *4* (8), 2123–2135. https://doi.org/10.1039/D5DD00069F.

Binte Mohamed, D. K.; Lapkin, A. A.; Wang, C.; Bu, J.; Tao, L.; Liu, W. Investigating the Kinetics of CO_2 Mineralization via the Carbonation of CaO in Ammonium Carbonate Solution by Reaction Heat Flow Calorimetry. *Ind. Eng. Chem. Res.* 2025, *64* (30), 14813–14828. https://doi.org/10.1021/acs.iecr.5c01369.

Chang, J.; Wang, S.; Hülsey, M. J.; Zhang, S.; Nee Lou, S.; Ma, X.; Yan, N. Electrothermal Conversion of Methane to Methanol at Room Temperature with Phosphotungstic Acid. *Angew Chem Int Ed* 2025, *64* (5), e202417251. https://doi.org/10.1002/anie.202417251.

Chen, J.; Bai, J.; Xu, J.; Farazi, F.; Mosbach, S.; Akroyd, J.; Kraft, M. Transforming Building Retrofits: Linking Energy, Equity, and Health Insights from The World Avatar. *Advances in Applied Energy* 2025, *19*, 100230. https://doi.org/10.1016/j.adapen.2025.100230.

Chen, Y.; Dai, C.; Wu, Q.; Li, H.; Xi, S.; Seow, J. Z. Y.; Luo, S.; Meng, F.; Bo, Y.; Xia, Y.; Jia, Y.; Fisher, A. C.; Xu, Z. J. Support-Free Iridium Hydroxide for High-Efficiency Proton-Exchange Membrane Water Electrolysis. *Nat Commun* 2025, *16* (1), 2730. https://doi.org/10.1038/s41467-025-58019-7.

Chen, Y.; Zheng, D. J.; Xu, Z. J.; Shao-Horn, Y. Best Practices for Oxygen Electrocatalysis. *Nat Sustain* 2024. https://doi.org/10.1038/s41893-024-01285-y.

Chin Law, L.; Gkantonas, S.; Mengoni, A.; Mastorakos, E. Onboard Pre-Combustion Carbon Capture with Combined-Cycle Gas Turbine Power Plant Architectures for LNG-Fuelled Ship Propulsion. *Applied Thermal Engineering* 2024, *248*, 123294. https://doi.org/10.1016/j.applthermaleng.2024.123294.

Chitre, A.; Cheng, J.; Ahamed, S.; Querimit, R. C. M.; Zhu, B.; Wang, K.; Wang, L.; Hippalgaonkar, K.; Lapkin, A. A. pHbot: Self-Driven Robot for pH Adjustment of Viscous Formulations via Physics-informed-ML**. *Chemistry Methods* 2024, *4* (2), e202300043. https://doi.org/10.1002/cmtd.202300043.

Chitre, A.; Querimit, R. C. M.; Rihm, S. D.; Karan, D.; Zhu, B.; Wang, K.; Wang, L.; Hippalgaonkar, K.; Lapkin, A. A. Accelerating Formulation Design via Machine Learning: Generating a High-Throughput Shampoo Formulations Dataset. *Sci Data* 2024, *11* (1), 728. https://doi.org/10.1038/s41597-024-03573-w.

Chitre, A.; Semochkina, D.; Woods, D. C.; Lapkin, A. A. Machine Learning-Guided Space-Filling Designs for High Throughput Liquid Formulation Development. *Computers & Chemical Engineering* 2025, *195*, 109007. https://doi.org/10.1016/j.compchemeng.2025.109007.

Dai, C.; Wu, Q.; Wu, T.; Zhang, Y.; Sun, L.; Wang, X.; Fisher, A. C.; Xu, Z. J. Suppressing Product Crossover and C–C Bond Cleavage in a Glycerol Membrane Electrode Assembly Reformer. *Energy Environ. Sci.* 2024, *17* (17), 6350–6359. https://doi.org/10.1039/D4EE01824A.

Deng, X.; Tsai, Y.; Ganguly, S.; Tran, D.; Quek, H. Y.; Ang, W.; Phua, S. Z.; Mosbach, S.; Akroyd, J.; Kraft, M. Question Answering System for Smart Cities and Urban Planning With The World Avatar. *IET Smart Cities* 2025, *7* (1), e70009. https://doi.org/10.1049/smc2.70009.

Duchon, M.; Matar, J.; Shoyari, M. F.; Perzylo, A.; Kessler, I.; Buchenberg, P.; Kuhn, P.; Hamacher, T.; Schlachter, T.; Süss, W.; Thinh, N. X.; Salari, H. E.; Latko, J.; Xu, M.; Shamovich, M.; Schlütter, D.; Frisch, J.; Rustagi, K.; Kraft, M.; Ayasse, C.; Steinke, F.; Metzger, M.; Kuper, L. A Platform Ecosystem Providing New Data For The Energy Transition. *SIGENERGY Energy Inform. Rev.* 2024, *4* (4), 226–237. https://doi.org/10.1145/3717413.3717435.

Eibeck, A.; Zhang, S.; Lim, M. Q.; Kraft, M. A Simple and Efficient Approach to Unsupervised Instance Matching and Its Application to Linked Data of Power Plants. *Journal of Web Semantics* 2024, *80*, 100815. https://doi.org/10.1016/j.websem.2024.100815.

Fan, Q.; Tan, M.; Yao, B.; Saqline, S.; Tao, L.; He, Q.; Liu, W. Synthesis of Uniform Fe2O3@Y2O3 Yolk–shell Nanoreactors as Chemical Looping Oxygen Carriers. *Applied Catalysis B: Environment and Energy* 2024, *350*, 123935. https://doi.org/10.1016/j.apcatb.2024.123935.

Fischer, A.; Bahry, T.; Xie, Z.; Qian, K.; Li, R.; Kwan, J.; Jerome, F.; Valange, S.; Liu, W.; Amaniampong, P.; Choksi, T. S. Harnessing Ultrasound-derived Hydroxyl Radicals for the Selective Oxidation of Aldehyde Functions. *ChemSusChem* 2024, e202400838. https://doi.org/10.1002/cssc.202400838.

Fischer, A. F.; Bahry, T.; Xie, Z.; da Silva Junior, R. B.; Qian, K.; Li, R.; Kwan, J.; Jerome, F.; Valange, S.; Liu, W.; Amaniampong, P. N.; Choksi, T. S. The Roles of Hydroxyl Radicals and Superoxide in Oxidizing Aqueous Benzyl Alcohol Under Ultrasound Irradiation. *ChemSusChem* 2025, e202500097. https://doi.org/10.1002/cssc.202500097.

Fulham, G. J.; Wu, X.; Liu, W.; Marek, E. J. Mechanistic Insights into the Role of Zinc Oxide, Zirconia and Ceria Supports in Cu-Based Catalysts for CO 2 Hydrogenation to Methanol. *Chemical Engineering Journal* 2024, *480*, 147732. https://doi.org/10.1016/j.cej.2023.147732.

Goh, D. Y. Y.; Yam, K. M.; Rekhi, L.; Handoko, A. D.; Tan, Y. C.; Wang, Y.; Tan, J. M. R.; Choksi, T. S.; Lum, Y.; Wong, L. H. Covalency-Aided Electrochemical CO_2 Reduction to CO on Sulfide-Derived Cu–Sb. *J. Mater. Chem. A* 2024, *12* (3), 1840–1851. https://doi.org/10.1039/D3TA04777F.

Hofmeister, M.; Bai, J.; Brownbridge, G.; Mosbach, S.; Lee, K. F.; Farazi, F.; Hillman, M.; Agarwal, M.; Ganguly, S.; Akroyd, J.; Kraft, M. Semantic Agent Framework for Automated Flood Assessment Using Dynamic Knowledge Graphs. *DCE* 2024, *5*, e14. https://doi.org/10.1017/dce.2024.11.

Hofmeister, M.; Brownbridge, G.; Hillman, M.; Mosbach, S.; Akroyd, J.; Lee, K. F.; Kraft, M. Cross-Domain Flood Risk Assessment for Smart Cities Using Dynamic Knowledge Graphs. *Sustainable Cities and Society* 2024, *101*, 105113. https://doi.org/10.1016/j.scs.2023.105113.

Hofmeister, M.; Lee, K. F.; Tsai, Y.-K.; Müller, M.; Nagarajan, K.; Mosbach, S.; Akroyd, J.; Kraft, M. Dynamic Control of District Heating Networks with Integrated Emission Modelling: A Dynamic Knowledge Graph Approach. *Energy and AI* 2024, *17*, 100376. https://doi.org/10.1016/j.egyai.2024.100376.

Jelinek, T.; Bhave, A.; Buchoud, N.; Bühler, M. M.; Glauner, P.; Inderwildi, O.; Kraft, M.; Mok, C.; Nübel, K.; Voss, A. International Collaboration: Mainstreaming Artificial Intelligence and Cyberphysical Systems for Carbon Neutrality. *Trans. Ind. Cyb-Phy. Sys.* 2024, *2*, 26–34. https://doi.org/10.1109/TICPS.2024.3351624.

Jia, Y.; Lu, Y.; Yang, H.; Chen, Y.; Hillman, F.; Wang, K.; Liang, C. Z.; Zhang, S. Control of Microporous Structure in Conjugated Microporous Polymer Membranes for Post-Combustion Carbon Capture. *Adv Funct Materials* 2024, 2407499. https://doi.org/10.1002/adfm.202407499.

Jorayev, P.; Soritz, S.; Sung, S.; Jeraal, M. I.; Russo, D.; Barthelme, A.; Toussaint, F. C.; Gaunt, M. J.; Lapkin, A. A. Machine Learning-Driven Optimization of Continuous-Flow Photoredox Amine Synthesis. *Org. Process Res. Dev.* 2025, *29* (6), 1411–1422. https://doi.org/10.1021/acs.oprd.4c00533.

Koh, S. W.; Rekhi, L.; Arramel; Birowosuto, M. D.; Trinh, Q. T.; Ge, J.; Yu, W.; Wee, A. T. S.; Choksi, T. S.; Li, H. Tuning the Work Function of MXene via Surface Functionalization. *ACS Appl. Mater. Interfaces* 2023, acsami.3c11857. https://doi.org/10.1021/acsami.3c11857.

Kondinski, A.; Mosbach, S.; Akroyd, J.; Breeson, A.; Tan, Y. R.; Rihm, S.; Bai, J.; Kraft, M. Hacking Decarbonization with a Community-Operated CreatorSpace. *Chem* 2024, S2451929423006198. https://doi.org/10.1016/j.chempr.2023.12.018.

Kondinski, A.; Oyarzún-Aravena, A. M.; Rihm, S. D.; Bai, J.; Mosbach, S.; Akroyd, J.; Kraft, M. Automated Assembly Modeling of Metal–Organic Polyhedra. *Eur J Inorg Chem* 2025, *28* (26), e202500115. https://doi.org/10.1002/ejic.202500115.

Kondinski, A.; Rutkevych, P.; Pascazio, L.; Tran, D. N.; Farazi, F.; Ganguly, S.; Kraft, M. Knowledge Graph Representation of Zeolitic Crystalline Materials. *Digital Discovery* 2024, 10.1039.D4DD00166D. https://doi.org/10.1039/D4DD00166D.

PUBLICATIONS

Kylikas, A.; Mastorakos, E. Simulations of Decane-Ammonia Autoignition in Two Mixture Fractions. *Front. Mech. Eng.* 2025, *10*, 1498820. https://doi.org/10.3389/fmech.2024.1498820.

Law, L. C.; Mastorakos, E.; Othman, Mohd. R.; Trakakis, A. A Thermodynamics Model for the Assessment and Optimisation of Onboard Natural Gas Reforming and Carbon Capture. *Emiss. Control Sci. Technol.* 2023. https://doi.org/10.1007/s40825-023-00234-z.

Liu, Y.; Harikrishnan, B.; Kolluru, R.; Mastorakos, E. Computational Fluid Dynamics Simulation of Ammonia Leakage Scenarios during Ship-to-Ship Bunkering. *Ocean Engineering* 2024, *312*, 119136. https://doi.org/10.1016/j.oceaneng.2024.119136.

Lu, Y.; Deng, H.; Zhang, L.; Wang, Y.; Zhang, S. Shape-Selective Molecular Separations Enabled by Rigid and Interconnected Confinements Engineered in Conjugated Microporous Polymer Membranes. *Advanced Science* 2025, *12* (22), 2416266. https://doi.org/10.1002/advs.202416266.

Luo, S.; Dai, C.; Ye, Y.; Wu, Q.; Wang, J.; Li, X.; Xi, S.; Xu, Z. J. Elevated Water Oxidation by Cation Leaching Enabled Tunable Surface Reconstruction. *Angew Chem Int Ed* 2024, *63* (31), e202402184. https://doi.org/10.1002/anie.202402184.

Ma, H.; Ye, X.; Li, X.; Xu, Z. J.; Sun, Y. Ferroelectric Polarization Effects of Single-Atom Catalysts on Water Oxidation. *Advanced Materials* 2025, 2500285. https://doi.org/10.1002/adma.202500285.

Ma, M.; Rivellini, L.-H.; Zong, Y.; Kraft, M.; Yu, L. E.; Lee, A. K. Y. Advances in Characterization of Black Carbon Particles and Their Associated Coatings Using the Soot-Particle Aerosol Mass Spectrometer in Singapore, a Complex City Environment. *Atmos. Chem. Phys.* 2025, *25* (14), 8185–8211. https://doi.org/10.5194/acp-25-8185-2025.

Meng, F.; Wu, Q.; Elouarzaki, K.; Luo, S.; Sun, Y.; Dai, C.; Xi, S.; Chen, Y.; Lin, X.; Fang, M.; Wang, X.; Mandler, D.; Xu, Z. J. Essential Role of Lattice Oxygen in Methanol Electrochemical Refinery toward Formate. *Sci. Adv.* 2023, *9* (34), eadh9487. https://doi.org/10.1126/sciadv.adh9487.

Ortiz, A.; López, S.; Ríos, A.; Copete, H.; Akroyd, J.; Mosbach, S.; Kraft, M.; Molina, A. Small-Scale Pyrometallurgical Plant for Recycling Spent Lead Acid Batteries: CFD Analysis of a Submerged Lance Furnace, Environmental and Economic Assessment, and Multiobjective Optimization. *Journal of Cleaner Production* 2025, *489*, 144654. https://doi.org/10.1016/j.jclepro.2025.144654.

Oyarzún-Aravena, A. M.; Chen, J.; Brownbridge, G.; Akroyd, J.; Kraft, M. An Analysis of Renewable Energy Resources and Options for the Energy Transition in Chile. *Applied Energy* 2025, *381*, 125107. https://doi.org/10.1016/j.apenergy.2024.125107.

Pascazio, L.; Rihm, S.; Naseri, A.; Mosbach, S.; Akroyd, J.; Kraft, M. Chemical Species Ontology for Data Integration and Knowledge Discovery. *J. Chem. Inf. Model.* 2023, *63* (21), 6569–6586. https://doi.org/10.1021/acs.jcim.3c00820.

Pham, T. T.; Guo, Z.; Li, B.; Lapkin, A. A.; Yan, N. Synthesis of Pyrrole-2-Carboxylic Acid from Cellulose- and Chitin-Based Feedstocks Discovered by the Automated Route Search. *ChemSusChem* 2024, *17* (3), e202300538. https://doi.org/10.1002/cssc.202300538.

Phua, S. Z.; Hofmeister, M.; Tsai, Y.-K.; Peppard, O.; Lee, K. F.; Courtney, S.; Mosbach, S.; Akroyd, J.; Kraft, M. Fostering Urban Resilience and Accessibility in Cities: A Dynamic Knowledge Graph Approach. *Sustainable Cities and Society* 2024, *113*, 105708. https://doi.org/10.1016/j.scs.2024.105708.

Phua, S. Z.; Lee, K. F.; Tsai, Y.-K.; Ganguly, S.; Yan, J.; Mosbach, S.; Ng, T.; Moise, A.; Horton, B. P.; Kraft, M. Urban Vulnerability Assessment of Sea Level Rise in Singapore through the World Avatar. *Applied Sciences* 2024, *14* (17), 7815. https://doi.org/10.3390/app14177815.

Quek, H. Y.; Hofmeister, M.; Rihm, S. D.; Yan, J.; Lai, J.; Brownbridge, G.; Hillman, M.; Mosbach, S.; Ang, W.; Tsai, Y.-K.; Tran, D. N.; Tan, S. K., William; Kraft, M. Dynamic Knowledge Graph Applications for Augmented Built Environments through "The World Avatar." *Journal of Building Engineering* 2024, *91*, 109507. https://doi.org/10.1016/j.jobe.2024.109507.

Rajagopalan, R.; Chaturvedi, S.; Chaudhary, N.; Gogoi, A.; Choksi, T. S.; Govind Rajan, A. Advances in CO_2 Reduction on Bulk and Two-Dimensional Electrocatalysts: From First Principles to Experimental Outcomes. *Current Opinion in Electrochemistry* 2025, *51*, 101668. https://doi.org/10.1016/j.coelec.2025.101668.

Rekhi, L.; Trinh, Q. T.; Prabhu, A. M.; Choksi, T. S. Generalized Principles for the Descriptor-Based Design of Supported Gold Catalysts. *ACS Catal.* 2024, *14* (18), 13839–13859. https://doi.org/10.1021/acscatal.4c04049.

Rihm, S. D.; Bai, J.; Kondinski, A.; Mosbach, S.; Akroyd, J.; Kraft, M. Transforming Research Laboratories with Connected Digital Twins. *Nexus* 2024, *1* (1), 100004. https://doi.org/10.1016/j.ynexs.2024.100004.

Rihm, S. D.; Saluz, F.; Kondinski, A.; Bai, J.; Butler, P. W. V.; Mosbach, S.; Akroyd, J.; Kraft, M. Extraction of Chemical Synthesis Information Using the World Avatar. *Digital Discovery* 2025, 10.1039.D5DD00183H. https://doi.org/10.1039/D5DD00183H.

Rihm, S. D.; Tan, Y. R.; Ang, W.; Hofmeister, M.; Deng, X.; Laksana, M. T.; Quek, H. Y.; Bai, J.; Pascazio, L.; Siong, S. C.; Akroyd, J.; Mosbach, S.; Kraft, M. The Digital Lab Manager: Automating Research Support. *SLAS Technology* 2024, *29* (3), 100135. https://doi.org/10.1016/j.slast.2024.100135.

Rihm, S. D.; Tan, Y. R.; Ang, W.; Quek, H. Y.; Deng, X.; Laksana, M. T.; Bai, J.; Mosbach, S.; Akroyd, J.; Kraft, M. The Digital Lab Facility Manager: Automating Operations of Research Laboratories through "The World Avatar." *Nexus* 2024, *1* (3), 100031. https://doi.org/10.1016/j.ynexs.2024.100031.

Rihm, S. D.; Tran, D. N.; Kondinski, A.; Pascazio, L.; Saluz, F.; Deng, X.; Mosbach, S.; Akroyd, J.; Kraft, M. Natural Language Access Point to Digital Metal–Organic Polyhedra Chemistry in The World Avatar. *DCE* 2025, *6*, e22. https://doi.org/10.1017/dce.2025.12.

Saqline, S.; Wang, H.; Fan, Q.; Donat, F.; Müller, C.; Liu, W. Investigation of Barium Iron Oxides for CO_2 Capture and Chemical Looping Oxygen Uncoupling. *Applications in Energy and Combustion Science* 2024, *17*, 100238. https://doi.org/10.1016/j.jaecs.2023.100238.

Shambhawi; Mohan, O.; Choksi, T. S.; Lapkin, A. A. The Design and Optimization of Heterogeneous Catalysts Using Computational Methods. *Catal. Sci. Technol.* 2024, *14* (3), 515–532. https://doi.org/10.1039/D3CY01160G.

Shao, D.; Wu, Q.; Zhang, Y.; Cai, X.; Dai, C.; Zhu, S.; Meng, F.; Song, P.; Li, X.; Ren, X.; Wu, T.; Xu, Z. J. Non-Linear Spin Correlation of Intermediates in Enhanced Electrochemical Nitrate Reduction under Magnetic Fields. *Energy Environ. Sci.* 2025, *18* (15), 7708–7719. https://doi.org/10.1039/D5EE02132D.

Shao, Y.; Wu, C.; Xi, S.; Tan, P.; Wu, X.; Saqline, S.; Liu, W. Halite-Structured (MgCoNiMnFe)O High Entropy Oxide (HEO) for Chemical Looping Dry Reforming of Methane. *Applied Catalysis B: Environment and Energy* 2024, *355*, 124191. https://doi.org/10.1016/j.apcatb.2024.124191.

Shen, Q.; Dai, C.; Liu, Y.; Zhang, Y.; Song, P.; Xi, P.; Xi, S.; Fisher, A. C.; Elouarzaki, K.; Xu, Z. J. Atomically Dispersed Zn and Ir Synergistic Modulation of Substrate and Active Sites for High-Performance Ammonia Oxidation. *Angewandte Chemie* 2025, *137* (39), e202513465. https://doi.org/10.1002/ange.202513465.

Sheng, Y.; Polynski, M. V.; Eswaran, M. K.; Zhang, B.; Lim, A. M. H.; Zhang, L.; Jiang, J.; Liu, W.; Kozlov, S. M. A Review of Mechanistic Insights into CO_2 Reduction to Higher Alcohols for Rational Catalyst Design. *Applied Catalysis B: Environmental* 2024, *343*, 123550. https://doi.org/10.1016/j.apcatb.2023.123550.

Siow, W. J. S.; Chong, J. Y.; Ong, J. H.; Kraft, M.; Wang, R.; Xu, R. Vapor/Vapor-Solid Interfacial Growth of Covalent Organic Framework Membranes on Alumina Hollow Fiber for Advanced Molecular Separation. *Angew Chem Int Ed* 2024, *63* (32), e202406830. https://doi.org/10.1002/anie.202406830.

Sun, L.; Dai, C.; Wang, T.; Jin, X.; Xu, Z. J.; Wang, X. Modulating the Electronic Structure of Cobalt in Molecular Catalysts via Coordination Environment Regulation for Highly Efficient Heterogeneous Nitrate Reduction. *Angew Chem Int Ed* 2024, *63* (15), e202320027. https://doi.org/10.1002/anie.202320027.

Sun, L.; Su, T.; Fisher, A. C.; Wang, X. Heterogeneous Electrochemical Carbon Dioxide Reduction in Aqueous Medium Using a Novel N4-Macrocyclic Cobalt Complex. *Small Methods* 2024, 2400627. https://doi.org/10.1002/smtd.202400627.

Sun, S.; Dai, C.; Zhao, P.; Xi, S.; Ren, Y.; Tan, H. R.; Lim, P. C.; Lin, M.; Diao, C.; Zhang, D.; Wu, C.; Yu, A.; Koh, J. C. J.; Lieu, W. Y.; Seng, D. H. L.; Sun, L.; Li, Y.; Tan, T. L.; Zhang, J.; Xu, Z. J.; Seh, Z. W. Spin-Related Cu-Co Pair to Increase Electrochemical Ammonia Generation on High-Entropy Oxides. *Nat Commun* 2024, *15* (1), 260. https://doi.org/10.1038/s41467-023-44587-z.

Tan, Y. R.; Hofmeister, M.; Phua, S. Z.; Brownbridge, G.; Rustagi, K.; Akroyd, J.; Mosbach, S.; Bhave, A.; Kraft, M. Beyond Connected Digital Twins – Can Digital Twins Really Deliver Sustainable Cities? *Sustainable Cities and Society* 2025, *131*, 106596. https://doi.org/10.1016/j.scs.2025.106596.

Tran, D.; Pascazio, L.; Akroyd, J.; Mosbach, S.; Kraft, M. Leveraging Text-to-Text Pretrained Language Models for Question Answering in Chemistry. *ACS Omega* 2024, *9* (12), 13883–13896. https://doi.org/10.1021/acsomega.3c08842.

Tsai, Y.-K.; Hofmeister, M.; Ganguly, S.; Rustagi, K.; Tan, Y. R.; Mosbach, S.; Akroyd, J.; Kraft, M. Municipal Heat Planning within The World Avatar. *Energy and AI* 2025, *20*, 100479. https://doi.org/10.1016/j.egyai.2025.100479.

Verma, A. K.; Atif, S.; Padhy, A.; Choksi, T. S.; Barpanda, P.; Govind Rajan, A. Robust Oxygen Evolution on Ni-Doped MoO_3: Overcoming Activity–Stability Trade-Off in Alkaline Water Splitting. *Chem Bio Eng.* 2025, cbe.4c00160. https://doi.org/10.1021/cbe.4c00160.

Wu, Q.; Dai, C.; Meng, F.; Jiao, Y.; Xu, Z. J. Potential and Electric Double-Layer Effect in Electrocatalytic Urea Synthesis. *Nat Commun* 2024, *15* (1), 1095. https://doi.org/10.1038/s41467-024-45522-6.

Wu, Q.; Shao, D.; Dai, C.; Wang, J.; Li, X.; Song, P.; Xie, W.; Xi, S.; Zhang, L.; Lin, X.; Luo, S.; Sun, S.; An, L.; Xi, P.; Xu, Z. J. Efficient Electrocatalytic Nitrate-to-Ammonia Enabled by Reversible Lattice-Oxygen Control. *J. Am. Chem. Soc.* 2025, *147* (33), 30401–30411. https://doi.org/10.1021/jacs.5c10362.

PUBLICATIONS

Wu, T.; Ge, J.; Wu, Q.; Ren, X.; Meng, F.; Wang, J.; Xi, S.; Wang, X.; Elouarzaki, K.; Fisher, A.; Xu, Z. J. Tailoring Atomic Chemistry to Refine Reaction Pathway for the Most Enhancement by Magnetization in Water Oxidation. *Proc. Natl. Acad. Sci. U.S.A.* 2024, *121* (19), e2318652121. https://doi.org/10.1073/pnas.2318652121.

Xie, W.; Atherton, J.; Bai, J.; Farazi, F.; Mosbach, S.; Akroyd, J.; Kraft, M. A Nuclear Future? Small Modular Reactors in a Carbon Tax-Driven Transition to Clean Energy. *Applied Energy* 2024, *364*, 123128. https://doi.org/10.1016/j.apenergy.2024.123128.

Xie, W.; Farazi, F.; Atherton, J.; Bai, J.; Mosbach, S.; Akroyd, J.; Kraft, M. Dynamic Knowledge Graph Approach for Modelling the Decarbonisation of Power Systems. *Energy and AI* 2024. https://doi.org/10.1016/j.egyai.2024.100359.

Xie, Z.; Mahendran, V.; Jonnalagadda, U. S.; Fan, Q.; Su, X.; Fischer, A. F.; Tan, M.; Tao, L.; Jérôme, F.; Kwan, J. J.; Valange, S.; Choksi, T. S.; Amaniampong, P. N.; Liu, W. Boosting Energy Efficiency and Selectivity of Glucose Oxidation toward Glucuronic Acid in High-Frequency Ultrasound Using Multicavity CuO Catalytic Cavitation Agents. *Green Chem.* 2025, *27* (3), 573–585. https://doi.org/10.1039/D4GC03775H.

Xu, J.; Mosbach, S.; Akroyd, J.; Kraft, M. Impact of Heat Pumps and Future Energy Prices on Regional Inequalities. *Advances in Applied Energy* 2025, *17*, 100201. https://doi.org/10.1016/j.adapen.2024.100201.

Ye, Y.; Wu, Q.; Xu, Z. J. Minireview on Decoding Electrocatalytic CO_2 Reduction via Lewis Acid–Base Chemistry: Advances and Outlook. *Energy Fuels* 2025, *39* (37), 17763–17778. https://doi.org/10.1021/acs.energyfuels.5c03374.

Zhang, C.; Arun, A.; Lapkin, A. A. Completing and Balancing Database Excerpted Chemical Reactions with a Hybrid Mechanistic-Machine Learning Approach. *ACS Omega* 2024, acsomega.4c00262. https://doi.org/10.1021/acsomega.4c00262.

Zhu, Q.; Zong, Y.; Tan, Y. R.; Lyu, J.-Y.; Pan, J.; Zhou, X.; Liu, H.; He, S.; Chen, W.; Yu, W.; Yang, W.; Kraft, M. Comparative Analysis of PODE3 and PODE4 Fuel Additives for Emission Reduction and Soot Characteristics in Compression Ignition Engines. *Energy* 2024, *286*, 129498. https://doi.org/10.1016/j.energy.2023.129498.

Zhu, Q.; Zong, Y.; Tan, Y. R.; Lyu, J.-Y.; Zhou, X.; Wu, Y.; Pan, J.; Liu, H.; He, S.; Chen, W.; Yu, W.; Yang, W.; Kraft, M. Reducing Particulate Matter Emissions and Investigating Soot Characteristics in CI Engines Using Alcohol-Based Additives: An Experimental Analysis. *International Journal of Hydrogen Energy* 2024, *87*, 10–19. https://doi.org/10.1016/j.ijhydene.2024.08.345.

Zhu, S.; Wu, Q.; Dai, C.; Yu, A.; Wu, T.; Ren, X.; Li, X.; Tadich, A.; Deng, D.; Liu, T.; Wu, Q.; Yue, M.; Xu, Z. J. Cooperative Spin Alignment Enhances Dimerization in the Electrochemical Ammonia Oxidation Reaction. *Nat. Chem.* 2025. https://doi.org/10.1038/s41557-025-01900-1.

CLIC: Centre for Lifelong Learning and Individualised Cognition

Friedman, N. P.; Robbins, T. W. The Role of Prefrontal Cortex in Cognitive Control and Executive Function. *Neuropsychopharmacol.* 2022, *47* (1), 72–89. https://doi.org/10.1038/s41386-021-01132-0.

Lee, L. Y.; Healy, M. P.; Fischer, N. L.; Tong, K.; Chen, A. S.; Sahakian, B. J.; Kourtzi, Z. Cognitive Flexibility Training for Impact in Real-World Settings. *Current Opinion in Behavioral Sciences* 2024, *59*, 101413. https://doi.org/10.1016/j.cobeha.2024.101413.

Leong, V.; Raheel, K.; Sim, J. Y.; Kacker, K.; Karlaftis, V. M.; Vassiliu, C.; Kalaivanan, K.; Chen, S. H. A.; Robbins, T. W.; Sahakian, B. J.; Kourtzi, Z. A New Remote Guided Method for Supervised Web-Based Cognitive Testing to Ensure High-Quality Data: Development and Usability Study. *J Med Internet Res* 2022, *24* (1), e28368. https://doi.org/10.2196/28368.

Melia, N.; Christopoulos, G.; Wigdorowitz, M.; Vassiliu, C.; Feng, S.; Abraham, A.; Chan, Y. N.; Lee, L. L.; Yap, H. S.; Robbins, T.; Sahakian, B.; Kourtzi, Z.; Leung, V.; Cheng, A.; Hendriks, H.; the CLIC Phase 1 Consortium. Validation of the CILD-Q for Measuring Contextual Linguistic Diversity in Singapore. *International Journal of Multilingualism* 2025, 1–18. https://doi.org/10.1080/14790718.2025.2570205.

Michael, E.; Covarrubias, L. S.; Leong, V.; Kourtzi, Z. Learning at Your Brain's Rhythm: Individualized Entrainment Boosts Learning for Perceptual Decisions. *Cerebral Cortex* 2022, bhac426. https://doi.org/10.1093/cercor/bhac426.

Teo, L. Z.; Leong, V. Age-Appropriate Adaptation of Creativity Tasks for Infants Aged 12–24 Months. *MethodsX* 2024, *12*, 102655. https://doi.org/10.1016/j.mex.2024.102655.

Tong, K.; Fu, X.; Hoo, N. P.; Kean Mun, L.; Vassiliu, C.; Langley, C.; Sahakian, B. J.; Leong, V. The Development of Cognitive Flexibility and Its Implications for Mental Health Disorders. *Psychol. Med.* 2024, 1–7. https://doi.org/10.1017/S0033291724001508.

Vassiliu, C.; Leong, V.; Hendriks, H. The Influence of Multilingual Experience on Executive Function and Structure Learning: Effects in Young Adults in the UK and Singapore. *Languages* 2024, *9* (4), 136. https://doi.org/10.3390/languages9040136.

Yu, J.; Fischer, N. L. Asymmetric Generalizability of Multimodal Brain-behavior Associations across Age-groups. *Human Brain Mapping* 2022, 1–12. https://doi.org/10.1002/hbm.26035.

Yu, J.; Fischer, N. L. Age-specificity and Generalization of Behavior-associated Structural and Functional Networks and Their Relevance to Behavioral Domains. *Human Brain Mapping* 2022, *43* (8), 2405–2418. https://doi.org/10.1002/hbm.25759.

Registered Studies

Feng, Shengchuang, George Christopoulos, Henriette Hendriks, Nadhilla Melia, Yoke Sam, Hui Shan Yap, Ke Tong, et al. 2022. 'Social Decision-Making and Its Association with Cognitive Flexibility in Healthy Young Adults', July. https://doi.org/10.17605/OSF.IO/JB38T.

Melani, Irene, George Christopoulos, Henriette Hendriks, Shengchuang Feng, Yoke Sam, Nadhilla Melia, Hui Shan Yap, et al. 2022. 'Cognitive Flexibility and Its Association with Linguistic Preferences, Decision-Making, Tolerance of Uncertainty and Perceived Social Support', August. https://doi.org/10.17605/OSF.IO/AY9GR.

Melia, Nadhilla, George Christopoulos, Henriette Hendriks, Shengchuang Feng, Yoke Sam, Hui Shan Yap, Ke Tong, et al. 2022. 'Tolerance of Uncertainty, Perceived Social Support, and Their Association with Structure Learning and Cognitive Flexibility in Healthy Young Adults', August. https://doi.org/10.17605/OSF.IO/SCJMP.

Sam, Yoke, George Christopoulos, SH Chen, Shengchuang Feng, Irene Melani, Nadhilla Melia, Henriette Hendriks, et al. 2022. 'Cognitive and Social Aspects of Career Transition and Adaptation', August. https://doi.org/10.17605/OSF.IO/N352U.

Tong, Ke, Ryutaro Uchiyama, Shengchuang Feng, Xiaoqin Cheng, Kastoori Kalaivanan, Victoria Leong, George Christopoulos, et al. 2022. 'Assessing Cognitive Flexibility, Other Executive Functions, and Learning in Healthy Young Adults', August. https://doi.org/10.17605/OSF.IO/6RC9H.

Uchiyama, Ryutaro, Nastassja Fischer, Phillis Fu, Timothy Lee, Xiaoqin Cheng, Shengchuang Feng, Irene Melani, et al. 2022. 'Assessing Cognitive Flexibility, Other Executive Functions, and Learning in Healthy Adolescents', August. https://doi.org/10.17605/OSF.IO/MD4TV.

Research Protocol papers

Liu, Chia-Lun, Xiaoqin Cheng, Boon Linn Choo, Min Hong, Jia Li Teo, Wei Ler Koo, Jia Yuan Janet Tan, et al. 2023. 'Potential Cognitive and Neural Benefits of a Computerised Cognitive Training Programme Based on Structure Learning in Healthy Adults: Study Protocol for a Randomised Controlled Trial'. *Trials* 24 (1): 517. https://doi.org/10.1186/s13063-023-07551-2.

Tong, Ke, Yuan Ni Chan, Xiaoqin Cheng, Bobby Cheon, Michelle Ellefson, Restria Fauziana, Shengchuang Feng, et al. 2023. 'Study Protocol: How Does Cognitive Flexibility Relate to Other Executive Functions and Learning in Healthy Young Adults?' Edited by Avanti Dey. *PLOS ONE* 18 (7): e0286208. https://doi.org/10.1371/journal.pone.0286208.

PhD thesis

Sam, Yoke Loo. 'Socio-Cognitive Aspects of Career Transition'. Nanyang Technological University, 2024. https://hdl.handle.net/10356/184212.

HD_4: Health-driven design for cities

Xu, Lei, Ronita Bardhan, Hao Mei, Srilalitha Gopalakrishnan, Xing Zheng, and Thomas Schroepfer. 'Harnessing Street Shade to Mitigate Heat Stress: An in-Situ Parallel Investigation under Extreme Heat Conditions in Tropical Singapore'. *Science of The Total Environment* 958 (January 2025): 177864. https://doi.org/10.1016/j.scitotenv.2024.177864.

PIPS

Hao, Zhimian, Magda H. Barecka, and Alexei A. Lapkin. 2022. 'Accelerating Net Zero from the Perspective of Optimizing a Carbon Capture and Utilization System'. *Energy & Environmental Science*, March, 10.1039.D1EE03923G. https://doi.org/10.1039/D1EE03923G.

Jeraal, Mohammed I., Simon Sung, and Alexei A. Lapkin. 2020. 'A Machine Learning-Enabled Autonomous Flow Chemistry Platform for Process Optimization of Multiple Reaction Metrics'. *Chemistry–Methods* 1 (1): 71–77. https://doi.org/10.1002/cmtd.202000044.

Karan, Dogancan, Guoying Chen, Nicholas Jose, Jiaru Bai, Paul McDaid, and Alexei A. Lapkin. 2024. 'A Machine Learning-Enabled Process Optimization of Ultra-Fast Flow Chemistry with Multiple Reaction Metrics'. *Reaction Chemistry & Engineering* 9 (3): 619–29. https://doi.org/10.1039/D3RE00539A.

Other publications

Jose, Nicholas, Mikhail Kovalev, Eric Bradford, Artur Schweidtmann, Hua Chun Zeng, and Alexei Lapkin. 2020. 'Pushing Nanomaterials Past the Kilogram Scale—a Targeted Approach Integrating Scalable Microreactors, Machine Learning and High-Throughput Analysis'. Preprint. https://doi.org/10.26434/chemrxiv.12732914.v1. [SMART—former project]

Schmidt, Hugo. 2019. 'Explosive Precursor Safety: An Application of the Deming Cycle for Continuous Improvement'. Journal of Chemical Health and Safety 26 (1): 31–36. https://doi.org/10.1016/j.jchas.2018.09.005. [Lab safety]

Schmidt, Hugo G. 2019. 'Use of Lean Six Sigma Methods to Eliminate Fume Hood Disorder'. Journal of Chemical Health and Safety, April, S1871553219300222. https://doi.org/10.1016/j.jchas.2019.03.006. [Lab safety]

C4T, CLIC, HYCOMBS, SM3, and HD4 are supported by the National Research Foundation, Prime Minister's Office, Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) programme.

PIPS Automated Evaluation of Environmental Impacts of Pharma Manufacturing Processes and Building a Capability in Magnetic Resonance Methods for the Pharmaceutical and Agrochemical Sector within PIPS is supported under the Pharmaceutical Innovation Programme Singapore.

AMPLE is supported by the National Research Foundation, Singapore, under its Central Gap Fund (Award NRF2020NRF-CG001-028).

LCER is supported by the National Research Foundation, Prime Minister's Office, Singapore under its Low-Carbon Energy Research (LCER) Phase 2 programme.

CAMBRIDGE CARES

cares.cam.ac.uk