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A COLLABORATION BETWEEN THE UNIVERSITY OF CAMBRIDGE,
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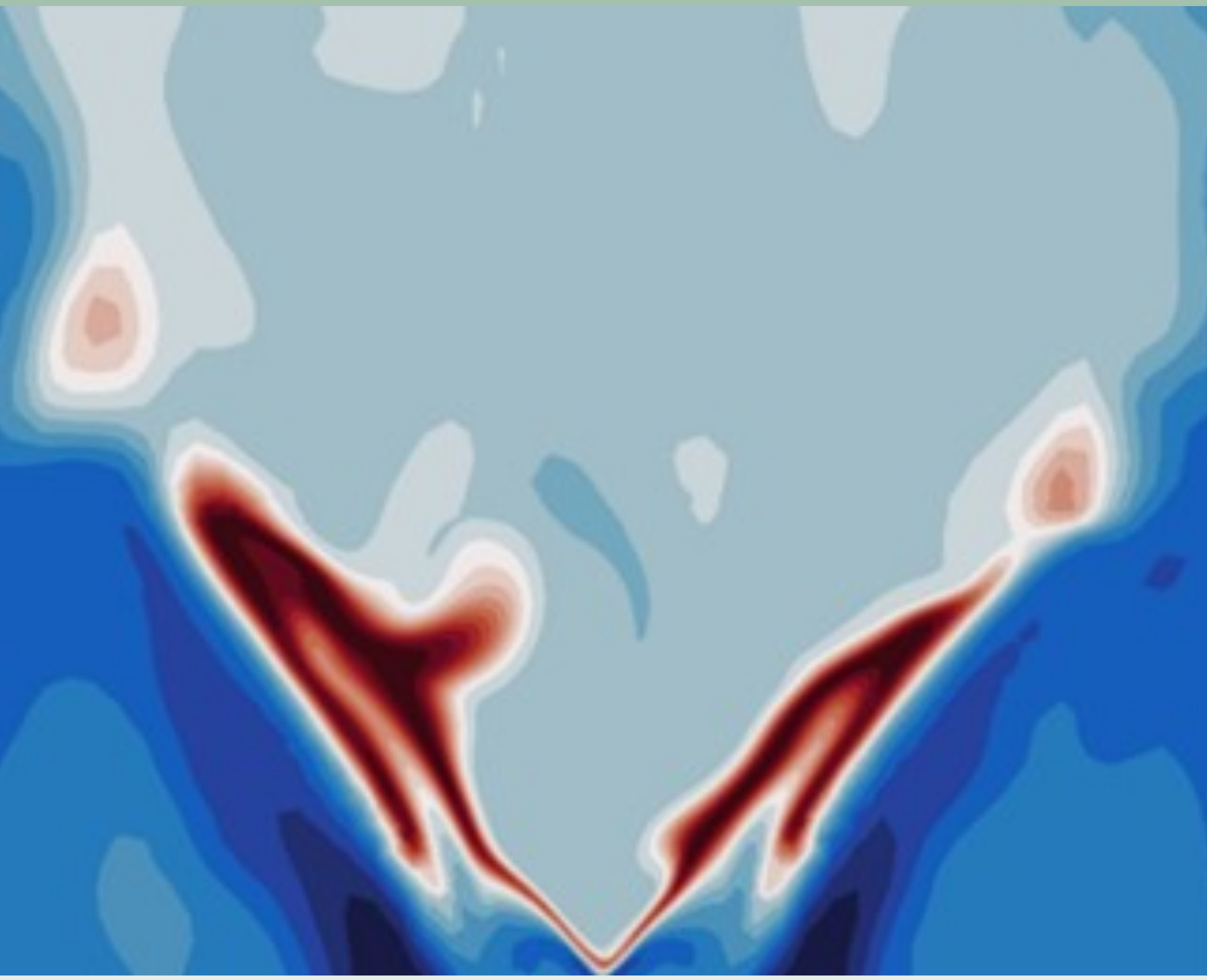

Biannual Research Report
April - September 2024

CAMBRIDGE
CARES

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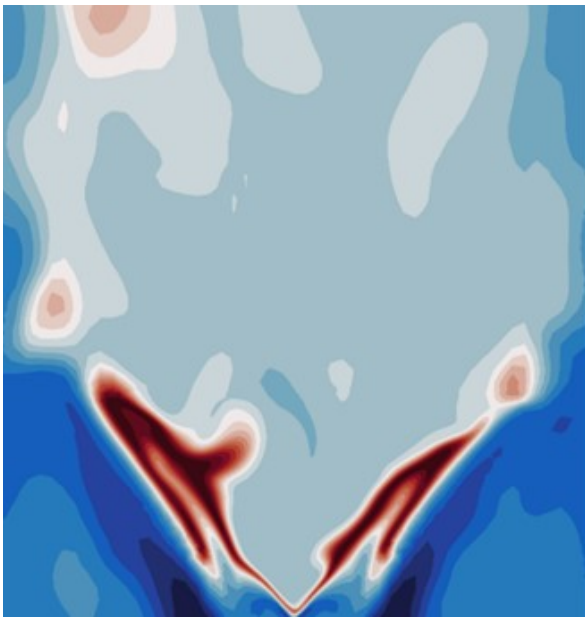
Cover image



Temperature field obtained from the in-house advanced turbulence-chemistry interaction solver, dcmcConverge, during a numerical investigation of n-heptane injected into a methane/air premixed gaseous mixture. The premixed mixture flows through a swirler before entering the combustion chamber through an annular passage. The image has been cropped for the cover.

Image by Dr B HARIKRISHNAN, CN14 Research Fellow. *See more on page 42.*

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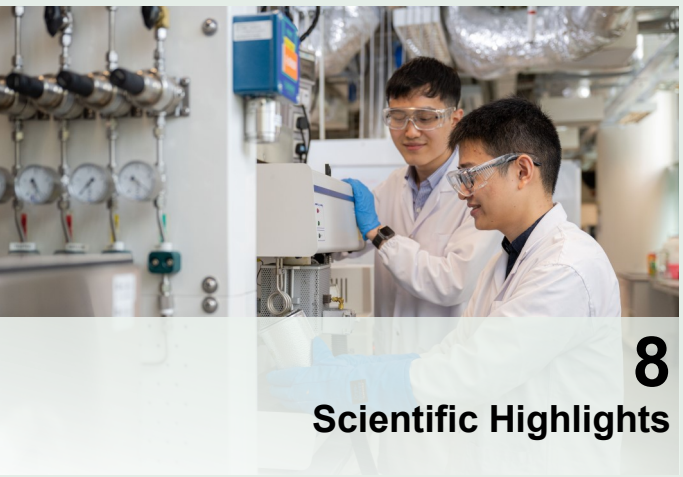

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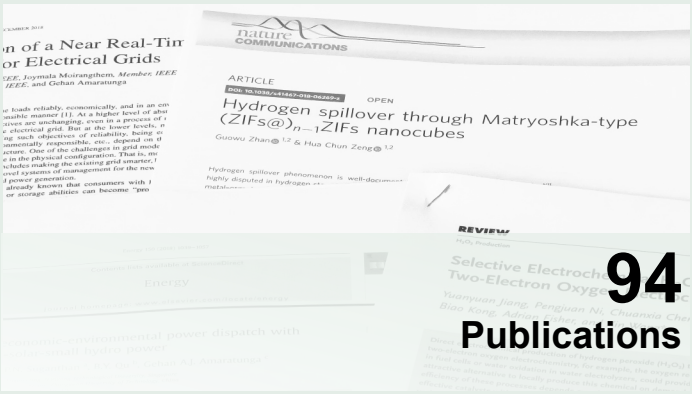

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FOREWORD

After 11 long years in Singapore, I take heart writing my last Director's Foreword for the CARES Biannual Research Reports. When we first thought of creating these reports back in 2014, I did not think there would be collectively 21 reports 5kg in weight to put in my suitcase as evidence of my time as Director. These reports were created for public transparency so that our research could be accessible, but they have also been a time capsule showcasing the longstanding research efforts from both our teams in Cambridge and Singapore. It has been a great joy to see how nascent programmes like Centre for Carbon Reduction in Chemical Technologies (C4T) have grown to support six start-ups, additional projects, and an international talent network in various fields. In addition, the Centre for Lifelong Learning and Individualised Cognition (CLIC) joining us in 2020 has certainly proven that CARES can act as a platform for diverse research opportunities. As we move forward, I would like to highlight a few exciting projects in the pipeline.

New projects in 2025

The foundation and network that C4T laid down has launched three new projects in the coming year. The first is Health-driven design for cities (HD_4) that will create a comprehensive systems view of how the urban environment affects population health, and two new projects in the SGD$90m Decarbonisation programme announced by the National Research Foundation in July 2024: Hydrogen and ammonia combustion in Singapore (HYCOMBS) and Sustainable Manufacture of Molecules and Materials in Singapore (SM_3). Progress on the new projects will be included in the next Biannual Report.

The Cambridge connection

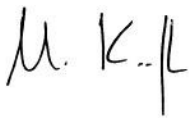
We have been entering exciting discussions with Cambridge HQ on how CARES can be leveraged by the University for South-East Asian activities. It was gratifying to hear Prof Deborah Prentice, Vice-Chancellor to the University of Cambridge, acknowledge CARES as a cornerstone for research and innovation at a recent Global Cambridge event in Singapore. While CARES has worked in the past closely with the University of Cambridge's Development and Alumni Relations (CUDAR) and Strategic Partnerships, we urge you to keep an eye on our social media for further activities in 2025.

Exploring creativity in Singapore

Following CLIC's *The Brainiverse Experience* outreach event in 2023, a creative spinoff in the form of an artbook was launched. The artworks from special needs students were compiled into a collection under the theme *Neurodiversity: No Brain is the Same* and is now available to view on our website: https://www.cares.cam.ac.uk/research/clic. Creativity and cognition are key themes of CLIC's research on lifelong learning—the additional perspective provided by the students was a wonderful learning experience.

I hope I have encouraged you to read more about CARES' latest work and achievements in this report. Please do get in touch if you would like to know more about our work or have ideas for collaboration.

Professor Markus Kraft, CARES Director
September 2024



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 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, and industrial partners.

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

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

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

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

CARES is currently hosting AMPLE (An Accelerated Manufacturing Platform for Engineered Nanomaterials), funded by the Central Gap Fund. AMPLE grew from research

within the C4T programme and is currently looking to bring their products to commercialisation via the spin-off company Accelerated Materials.

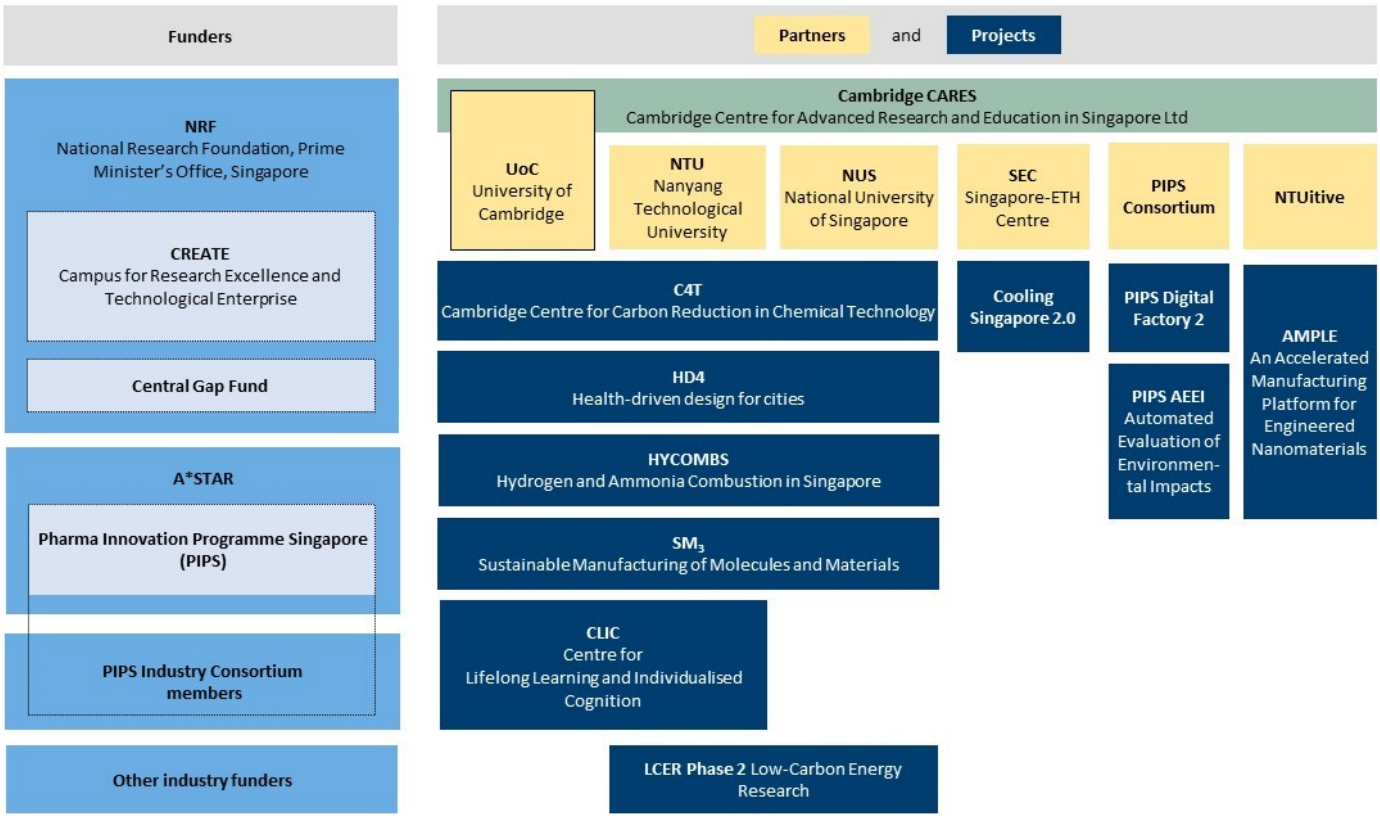
There are currently two ongoing streams under the Pharmaceutical Innovation Programme Singapore (PIPS); one stream builds on CARES work on a previous PIPS project to create a methodology for digital twins for pharmaceutical process development, another stream will focus on using data-driven solutions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

CARES is contributing to the Cooling Singapore 2.0 programme hosted by the Singapore-ETH Centre and two projects in the Low-Carbon Energy Research (LCER) Phase 2 Programme, one hosted by NUS and one hosted by NTU. Details and updates for these smaller projects can be found on page 87.

CARES will be hosting three new projects that will be included in the next report: Health-driven design for cities (HD_4), Hydrogen and ammonia combustion in Singapore (HYCOMBS), and Sustainable Manufacture of Molecules and Materials in Singapore (SM_3).

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

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



HIGHLIGHTS

OUTSTANDING WORK FROM THE LAST SIX MONTHS OF CAMBRIDGE CARES RESEARCH

Highlighted research outputs from April - September 2024

A selection of publications from across our programmes.

C4T: Accelerating Formulation Design via Machine Learning: Generating a High-throughput Shampoo Formulations Dataset

Aniket Chitre, Robert C. M. Querimit, Simon D. Rihm, Dogancan Karan, Benchuan Zhu, Ke Wang, Long Wang, Kedar Hippalgaonkar, and Alexei Lapkin, *Scientific Data*

DOI: 10.1038/s41597-024-03573-w

Abstract: Liquid formulations are ubiquitous yet have lengthy product development cycles owing to the complex physical interactions between ingredients making it difficult to tune formulations to customer-defined property targets. Interpolative ML models can accelerate liquid formulations design but are typically trained on limited sets of ingredients and without any structural information, which limits their out-of-training predictive capacity. To address this challenge, we selected eighteen formulation ingredients covering a diverse chemical space to prepare an open experimental dataset for training ML models for rinse-off formulations development. The resulting design space has an over 50-fold increase in dimensionality compared to our previous work. Here, we present a dataset of 812 formulations, including 294 stable samples, which cover the entire design space, with phase stability, turbidity, and high-fidelity rheology measurements generated on our semi-automated, ML-driven liquid formulations workflow. Our dataset has the unique attribute of sample-specific uncertainty measurements to train predictive surrogate mod-

C4T: Harnessing ultrasound-derived hydroxyl radicals for the selective oxidation of aldehyde functions

Ari Fischer, Teseer Bahry, Zhangyue Xie, Kaicheng Qian, Renhong Li, James Kwan, François Jerome, Sabine Valange, Wen Liu, Prince Amaniampong, and Tej S Choksi, *ChemSusChem*

DOI: 10.1002/cssc.202400838

Abstract: Ultrasonic irradiation holds potential for the selective oxidation of non-volatile organic substrates in the aqueous phase by harnessing hydroxyl radicals as chemical initiators. Here, a mechanistic description of hydroxyl radical-initiated glyoxal oxidation is constructed by gleaning insights from photolysis and radiation chemistry to explain the yields and kinetic trends for oxidation products. The mechanistic description and kinetic measurements reported herein reveal that increasing the formation rate of hydroxyl radicals by changing the ultrasound frequency increases both the rates of glyoxal consumption and the selectivity towards C2 acid products over those from C-C cleavage. Glyoxal consumption also occurs more rapidly and with greater selectivity towards C2 acids under acidic conditions, which favor the protonation of carboxylate intermediates into their less reactive acidic forms. Leveraging such pH and frequency effects is crucial to mitigating product degradation by secondary reactions with hydroxyl radicals and oxidation products (specifically hydrogen peroxide and superoxide). These findings demonstrate the potential of ultrasound as a driver for the selective oxidation of aldehyde functions to carboxylic acids, offering a sustainable route for valorizing biomass-derived platform molecules.

C4T: Semantic agent framework for automated flood assessment using dynamic knowledge graphs

Markus Hofmeister, Jiaru Bai, George Brownbridge, Sebastian Mosbach, Kok F. Lee, Feroz Farazi, Michael Hillman, Mehal Agarwal, Srishti Ganguly, Jethro Akroyd, and Markus Kraft, *Data-Centric Engineering*

DOI: 10.1017/dce.2024.11

Abstract: This article proposes a framework of linked software agents that continuously interact with an underlying knowledge graph to automatically assess the impacts of potential flooding events. It builds on the idea of connected digital twins based on the World Avatar dynamic knowledge graph to create a semantically rich asset of data, knowledge, and computational capabilities accessible to humans, applications, and artificial intelligence. We develop three new ontologies to describe and link environmental measurements and their respective reporting stations, flood events, and their potential impact on population and built infrastructure as well as the built environment of a city itself. These coupled ontologies are deployed to dynamically instantiate near real-time data from multiple fragmented sources into the World Avatar. Sequences of autonomous agents connected via the derived information framework automatically assess consequences of newly instantiated data, such as newly raised flood warnings, and cascade respective updates through the graph to ensure up-to-date insights into the number of people and building stock value at risk. Although we showcase the strength of this technology in the context of flooding, our findings suggest that this system-of-systems approach is a promising solution to build holistic digital twins for various other contexts and use cases to support truly interoperable and smart cities.

C4T: International Collaboration: Mainstreaming Artificial Intelligence and Cyberphysical Systems for Carbon Neutrality

Thorsten Jelinek, Amit Bhave, Nicolas Buchoud, Michael Max Bühler, Patrick Glauner, Oliver Inderwildi, Markus Kraft, Charles Mok, Konrad Nübel, and Alex Voss, *IEEE Transactions on Industrial Cyber-Physical Systems*

DOI: 10.1109/TICPS.2024.3351624

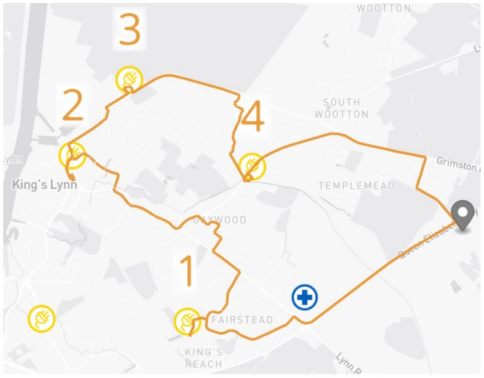
Abstract: Cyberphysical systems together with Artificial Intelligence play vital roles in reducing, eliminating, and removing greenhouse gas emissions across sectors. Electrification with renewables introduces complexity in systems in the deployment, integration, and efficient orchestration of electrified economic systems. AI-driven cyberphysical systems are uniquely suited to tackle this complexity, potentially accelerating the transition towards a low-carbon economy. The objective of this policy brief is to advocate for the mainstreaming of AI-driven cyberphysical systems for climate change risk mitigation and adaptation. To effectively and more rapidly realize the Intelligent Decarbonation potential, the concept of AI-driven cyberphysical systems must be elevated to a global level of collaboration and coordination, fostering research and development, capacity building, as well as knowledge and technology transfer. Drawing on a multidisciplinary, international study about intelligent decarbonization use cases, this brief also highlights factors impeding the transition to carbon neutrality and risks associated with technology determinism. The importance of governance is emphasized to avoid unwanted path dependency and avert a technology-solutionist approach dominating climate policy that delivers limited results. Given only 12% of the Sustainable Development Goals have been realized, a condensed version of this policy brief was submitted to the India T20, a G20 engagement group, urging global collaboration to prioritize AI-driven CPSs.

C4T: Fostering urban resilience and accessibility in cities: A dynamic knowledge graph approach

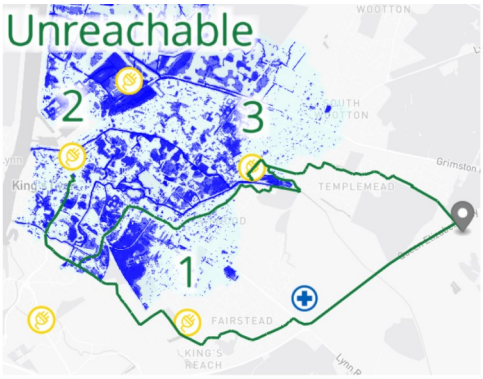
Shin Zert Phua, Markus Hofmeister, Yi-Kai Tsai, Oisín Peppard, Kok Foong Lee, Seán Courtney, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *Sustainable Cities and Society*

DOI: 10.1016/j.scs.2024.105708

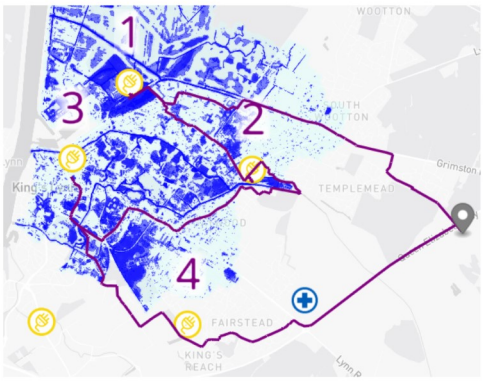
Abstract: This paper explores the utilisation of knowledge graphs and an agent-based implementation to enhance urban resilience and accessibility in city planning. We expand The World Avatar (TWA) dynamic knowledge graph to support decision-making in disaster response and urban planning. By employing a set of connected agents and integrating diverse data sources — including flood data, geospatial building information, land plots, and open-source data — through sets of ontologies, we demonstrate disaster response in a coastal town in the UK and various aspects relevant to city planning for a mid-sized town in Germany using TWA. In King's Lynn, our agent-based approach facilitates holistic disaster response by calculating optimal routes, avoiding flooded segments dynamically, assessing infrastructure accessibility before and during a flood using isochrones, identifying inaccessible population areas, guiding infrastructure restoration, and conducting critical path analysis. In Pirmasens, for city planning purposes, the knowledge graph-driven isochrone generation provides evidence-based insights into current amenity coverage and enables scenario planning for future amenities while adhering to land regulations. The implementation of agents and knowledge graphs achieves interoperability and enhances urban resilience and accessibility by enabling cross-domain correlation analysis that extends various areas including geospatial buildings, population demographics, accessibility coverage, and land use regulations.



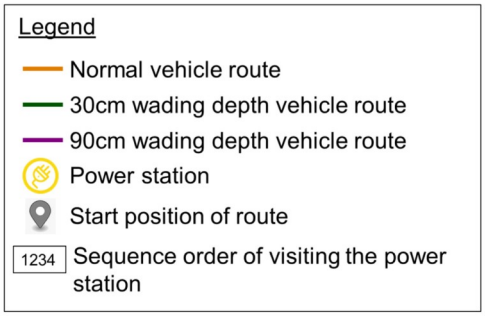
(a) Normal road conditions



(b) Flooded conditions: Deployment of 30cm wading depth vehicle



(c) Flooded conditions: Deployment of 90cm wading depth vehicle



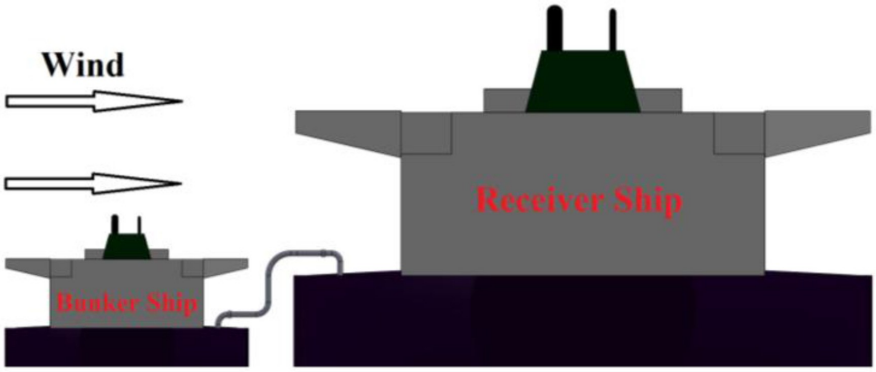
C4T: Computational fluid dynamics simulation of ammonia leakage scenarios during ship-to-ship bunkering

Yangyang Liu, B. Harikrishnan, Ramesh Kolluru, and Epaminondas Mastorakos, *Ocean Engineering*

DOI: 10.1016/j.oceaneng.2024.119136

Abstract: Ammonia is emerging as a potential marine fuel, yet its toxicity and risk of accidental leaks pose significant safety challenges compared to other alternatives. This study focuses on the critical ship-to-ship bunkering process using Computational Fluid Dynamics (CFD) simulations to analyse diverse ammonia leakage scenarios considering various leak orientations relative to the wind and the ships. The numerical setup was initially validated against controlled experiments, demonstrating satisfactory agreement. Results indicate that atmospheric ammonia dispersion is significantly influenced by obstacles like the superstructure and hull in the near field, with diminishing effect in the far field. Conventional Gaussian plume models are inadequate within the first few hundred metres from the release source due to the complex near-field flow patterns and increased turbulence generated by the wakes of the hull and superstructure. These findings underscore the necessity for improved ship-scale dispersion models to accurately evaluate the impact of obstacles on ammonia dispersion. The consequence analysis reveals that upward leaks create larger risk zones with potential for irreversible health effects, while horizontal leaks may expose personnel to life-threatening concentrations. Vertical leaks in crosswind configurations generate lethal zones covering tens of metres on deck. These results highlight the importance of considering the exact location of the transfer hose relative to the ship and all potential wind orientations in risk assessments. Given the extensive range of potential dispersion patterns and the inadequacy of conventional Gaussian dispersion models in this context, we strongly recommend vessel-specific CFD simulations before certifying ammonia bunkering operations as safe. This approach is crucial for accurate risk assessment at the ship scale, where complex geometries and multi-directional flows invalidate the assumptions of traditional point-source, unidirectional dispersion models.

(a)



(b)

C4T: Control of Microporous Structure in Conjugated Microporous Polymer Membranes for Post-Combustion Carbon Capture

Yuewen Jia, Yanqiu Lu, Haozhou Yang, Yu Chen, Febrian Hillman, Kaiyu Wang, Can Zeng Liang, and Sui Zhang, *Advanced Functional Materials*

DOI: 10.1002/adfm.202407499

Abstract: Membranes offer a potentially energy-efficient and space-saving solution to reduce CO2 emissions and combat global warming. However, engineering membranes with advanced materials for high permeance and reasonable selectivity is a pressing need. In this context, a series of carbazole-based conjugated microporous polymer (CMP) membranes are fabricated with thicknesses of a few hundred nanometers through in situ electropolymerization for post-combustion carbon capture. The findings reveal that various experimental conditions, including the monomer concentration, electric potential, and cyclic voltammetry (CV) cycling number, largely impact the polymerization degree of the carbazole-based CMP, thus influencing the mode of polymer chain packing. An optimal polymerization degree leads to a larger micropore size and a higher fractional free volume (FFV), thus allowing fast CO2 transport. The study first demonstrates the feasibility of using CMPs to fabricate thin film composite (TFC) membranes for post-combustion carbon capture and confirms the high controllability of their micropores. These insights provide instructive guidance for the future advancement of CMP applications in membrane fabrication for gas separation and other fields that require precise micropore

C4T: The Digital Lab Facility Manager: Automating operations of research laboratories through "The World Avatar"

Simon D. Rihm, Yong Ren Tan, Wilson Ang, Hou Yee Quek, Xinhong Deng, Michael Teguh Laksana, Jiaru Bai, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *Nexus*

DOI: 10.1016/j.ynexs.2024.100031

Abstract: This paper presents a novel framework for digitalizing and automating the management of specialized research laboratories using The World Avatar, a general all-encompassing dynamic knowledge graph. Semantic Web technology empowers users to effectively utilize data across various systems and formats without restricting them to a single software or protocol. Employing agents and ontologies, it enables seamless data sharing, computational reasoning, and gradual automation of tasks, addressing obstacles in interoperability and adaptability. Showcasing the capabilities of this approach, we tackle some common challenges in lab facility management, including cost-effective Internet of Things (IoT) sensor network integration with an existing building management system and efficient airflow management for fume hoods via "human-in-the-loop" interventions. We also develop unified platform-agnostic interfaces that complement the framework. These advancements represent a significant stride in the holistic digitalization and automation of research laboratories at the nexus of fundamental science and smart building applications, setting a foundation for future research facilities to achieve operational excellence and sustainability.

C4T: A review of mechanistic insights into CO2 reduction to higher alcohols for rational catalyst design

Yao Sheng, Mikhail V. Polynski, Mathan K. Eswaran, Bikun Zhang, Alvin M.H. Lim, Lili Zhang, Jianwen Jiang, Wen Liu, and Sergey M. Kozlov, *Applied Catalysis B: Environmental*

DOI: 10.1016/j.apcatb.2023.123550

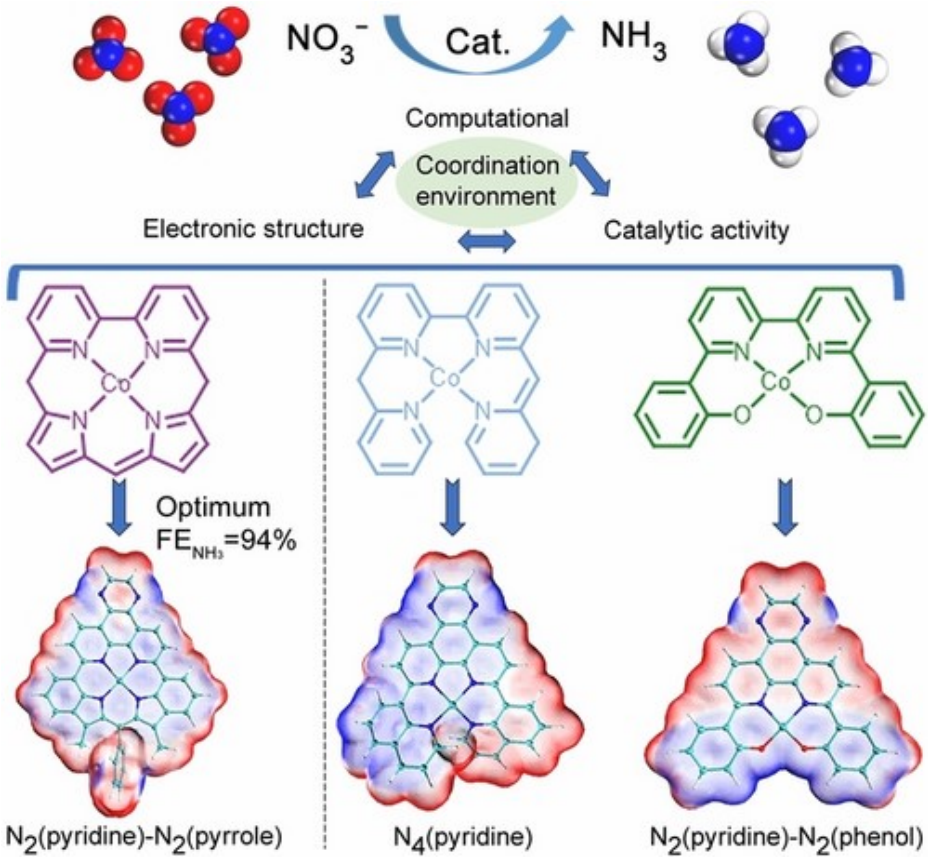
Abstract: The utilization of captured CO_2 for chemical synthesis could play an important role in reducing CO_2 emissions. Higher alcohols stand out among various products of CO_2 reduction due to high market prices and diverse applications, e.g., as fuel additives. However, developing catalysts for this reaction requires a profound understanding of the reaction mechanisms and catalyst design principles, which are discussed in the present review. Depending on the catalytic sites, higher alcohol synthesis could proceed via vastly different pathways. Herein, we outline how various proposed reaction mechanisms lead to different catalyst design strategies for optimizing the rate of CO_2 conversion into reactive C_1 intermediates (CO, CH_x, CH_xO, and HCOO) and their coupling into C_{2+} intermediates that are eventually converted into higher alcohols. Lastly, we discuss knowledge gaps in achieving rational catalyst design for higher alcohol synthesis and the breakthrough potential of machine-learning techniques for catalyst discovery.

C4T: Modulating the Electronic Structure of Cobalt in Molecular Catalysts via Coordination Environment Regulation for Highly Efficient Heterogeneous Nitrate Reduction

Libo Sun, Chencheng Dai, Tianjiao Wang, Xindie Jin, Zhichuan J. Xu, and Xin Wang , *Angewandte Chemie International Edition*

DOI: https://doi.org/10.1002/anie.202320027.

Abstract: Ammonia (NH_3) is pivotal in modern industry and represents a promising next-generation carbon-free energy carrier. Electrocatalytic nitrate reduction reaction (eNO_3RR) presents viable solutions for NH_3 production and removal of ambient nitrate pollutants. However, the development of eNO_3RR is hindered by lacking the efficient electrocatalysts. To address this challenge, we synthesized a series of macrocyclic molecular catalysts for the heterogeneous eNO_3RR. These materials possess different coordination environments around metal centers by surrounding subunits. Consequently, electronic structures of the active centers can be altered, enabling tunable activity towards eNO_3RR. Our investigation reveals that metal center with an N_2(pyrrole)-N_2(pyridine) configuration demonstrates superior activity over the others and achieves a high NH_3 Faradaic efficiency (FE) of over 90 % within the tested range, where the highest FE of approximately 94 % is obtained. Furthermore, it achieves a production rate of 11.28 mg mg_{cat}^{-1} h^{-1}, and a turnover frequency of up to 3.28 s^{-1}. Further tests disclose that these molecular catalysts with diverse coordination environments showed different magnetic moments. Theoretical calculation results indicate that variated coordination environments can result in a d-band center variation which eventually affects rate-determining step energy and calculated magnetic moments, thus establishing a correlation between electronic structure, experimental activity, and computational parameters.

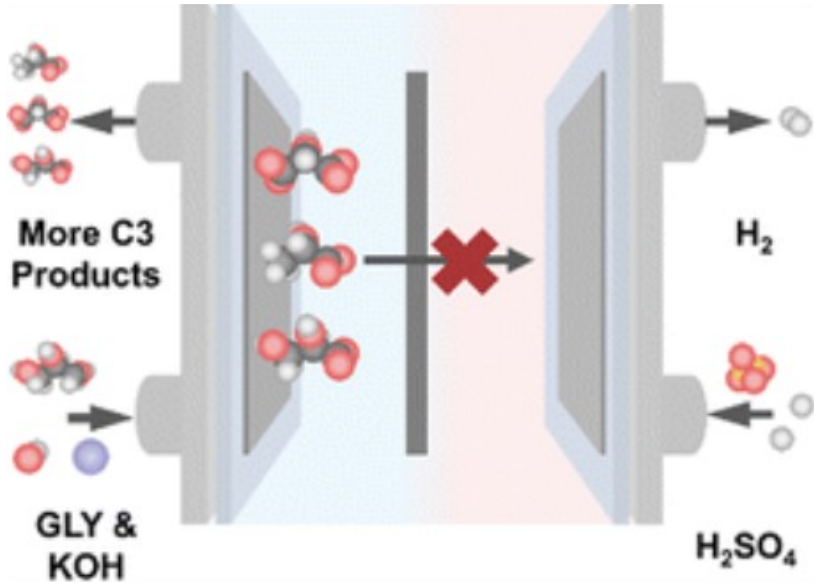


C4T: Suppressing product crossover and C–C bond cleavage in a glycerol membrane electrode assembly reformer†

Chencheng Dai, Qian Wu, Tianze Wu, Yuwei Zhang, Libo Sun, Xin Wang, Adrian C. Fisher, and Zhichuan J. Xu, *Energy & Environmental Science*

DOI: 10.1039/D4EE01824A

Abstract: Generating hydrogen through water electrolysis is impeded by high costs and substantial energy consumption mainly due to high equilibrium potential and sluggish kinetics of the oxygen evolution reaction (OER). Glycerol oxidation reaction (GOR) is proposed as an alternative due to its low thermodynamic limit and value-added oxidation products. However, GOR in membrane electrolyzers faces challenges in achieving industrial-scale current densities as well as in addressing crossover issues. Here, we investigated five different membrane electrode assembly (MEA) configurations to perform GOR with various ion exchange membranes and catholyte. After systematic study, we present an innovative acid–alkali asymmetric cell design which operates with alkaline anolyte and acidic catholyte for electrochemical neutralization energy (ENE) harvesting to improve energy efficiency. The product anions crossover *via* anion exchange membrane (AEM) is also impeded since that the increasing concentration gradient-driven hydroxide ion crossover occupying the anion exchange channels in AEM and thus limits the product crossover of AEM. Such device also demonstrates the capability of impeding C–C bond cleavage to promote high-value C3 products generation and reduce carbon emission due to the lower degree of cell polarization and limited hydroxide ion supply at anode. Eventually, a whole-cell potential can be significantly reduced to 0.377 V while achieving a current density of 200 mA cm^{-2}. Moreover, total faradaic efficiencies (FEs) of 55% and 84% for all C3 products and all liquid products can be achieved at a current density up to 1000 mA cm^{-2}.



C4T: Completing and Balancing Database Excerpted Chemical Reactions with a Hybrid Mechanistic-Machine Learning Approach

Chonghuan Zhang, Adarsh Arun, and Alexei Lapkin, *ACS Omega*

DOI: 10.1021/acsomega.4c00262

Abstract: Computer-aided synthesis planning (CASP) development of reaction routes requires an understanding of complete reaction structures. However, most reactions in the current databases are missing reaction coparticipants. Although reaction prediction and atom mapping tools can predict major reaction participants and trace atom rearrangements in reactions, they fail to identify the missing molecules to complete reactions. This is because these approaches are data-driven models trained on the current reaction databases, which comprise incomplete reactions. In this work, a workflow was developed to tackle the reaction completion challenge. This includes a heuristic-based method to identify balanced reactions from reaction databases and complete some imbalanced reactions by adding candidate molecules. A machine learning masked language model (MLM) was trained to learn from simplified molecular input line entry system (SMILES) sentences of these completed reactions. The model predicted missing molecules for the incomplete reactions, a workflow analogous to predicting missing words in sentences. The model is promising for the prediction of small- and middle-sized missing molecules in incomplete reaction records. The workflow combining both the heuristic and machine learning methods completed more than half of the entire reaction space.

CLIC: Cognitive flexibility training for impact in real-world settings

Liz Y Lee, Máiréad P Healy, Nastassja L Fischer, Ke Tong, Annabel SH Chen, Barbara J Sahakian, and Zoe Kourtzi, *Current Opinion in Behavioral Sciences*

DOI: 10.1016/j.cobeha.2024.101413

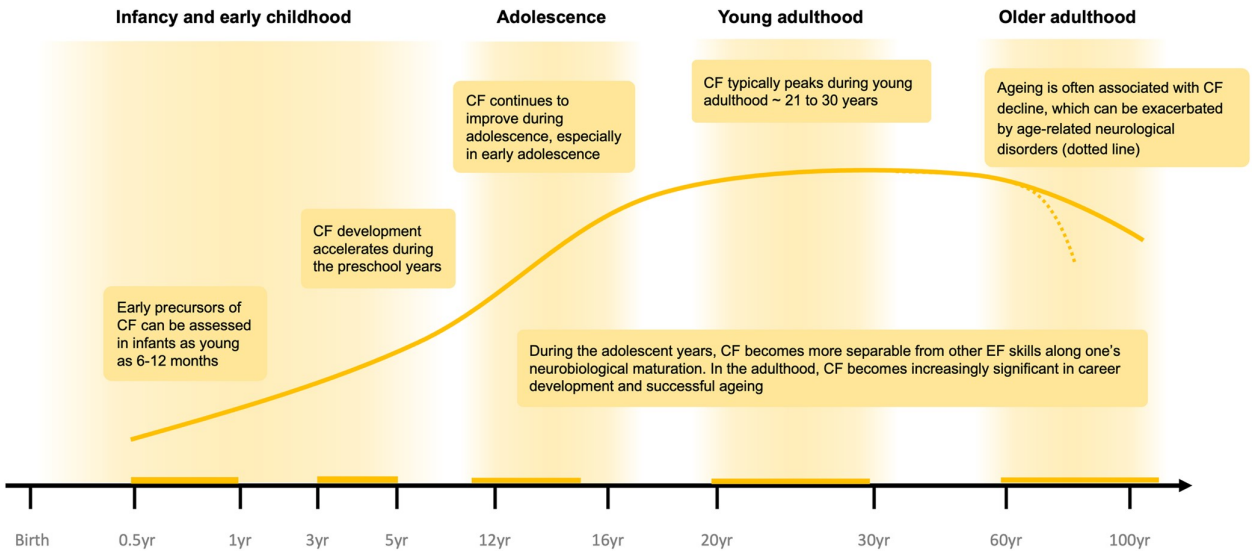
Abstract: Interacting with complex and dynamic environments challenges the brain's ability to adapt to change. This key ability known as cognitive flexibility involves learning the structure of the environment, switching attention between features, dimensions and tasks, and adopting new rules in the face of uncertainty. Training cognitive flexibility has strong potential to improve adaptive behavior across the lifespan with impact in real-world settings (e.g. educational, clinical). Here, we review evidence on the role of cognitive training in improving executive functions and the factors that may enhance the effectiveness of training programs. We propose that personalized and adaptive training programs that focus on the multifaceted abilities comprising cognitive flexibility are key for promoting adaptive behavior and lifelong learning in real-world settings.

CLIC: The development of cognitive flexibility and its implications for mental health disorders

Ke Tong, Xinchen Fu, Natalie P. Hoo, Lee Kean Mun, Chrysoula Vassiliu, Christelle Langley, Barbara J. Sahakian, and Victoria Leong, *Psychological Medicine*

DOI: 10.1017/S0033291724001508

Abstract: Cognitive flexibility (CF) represents the ability to adapt one's thinking and behavior in response to changing environmental demands (Uddin, 2021). CF is multifaceted and involves a range of skills, including attentional shifting, strategy updating, response to feedback, reversal learning, exploration, and task switching. As a core component of executive function (EF), CF works in tandem with working memory and inhibitory control to facilitate goal-oriented behavior (Friedman & Robbins, 2022). However, this editorial will focus on the development of CF and its implications for mental health disorders. CF is also impaired in a number of mental health disorders, including autism spectrum disorder (ASD) (Hughes, Russell, & Robbins, 1994), obsessive-compulsive disorder (OCD) (Gottwald et al., 2018; Vaghi et al., 2017), and schizophrenia (Murray et al., 2008). CF exhibits a prolonged maturational developmental trajectory, although early precursors of these skills can already be measured from infancy. The image below provides a graphical illustration of the lifespan trajectory of CF development during infancy, adolescence, young adulthood, and older adulthood. This is also important considering that many mental health disorders begin in childhood and adolescence. Here, we discuss key environmental factors that may be important for shaping CF development across different life stages and their implications for mental health.



C4T

CAMBRIDGE CENTRE FOR CARBON REDUCTION IN CHEMICAL TECHNOLOGIES (C4T)

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

C4T leads:

Professor Markus KRAFT
University of Cambridge

Professor Rong XU
Nanyang Technological University

Professor Ning YAN
National University of Singapore

SUSTAINABLE REACTION ENGINEERING

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

Asst Prof Wen LIU (Paul) (NTU)

Asst Prof Tej CHOKSI (NTU)

Ms Xianyue WU (Research Assistant, CARES) has been actively working on the development of CO_2 capture and in-situ hydrogenation process using Ni/alkaline earth metal carbonate dual-function materials (DFMs). She has been investigating mechanistic and kinetics studies on the hydrogenation of the Ni-amorphous $CaCO_3$-based dual-function materials (DFMs). She studied the effects of H_2 partial pressure on the hydrogenation of Ni/$CaCO_3$ DFM (Figure 1.1), and the decomposition of carbonate species during the process (Figure 1.2). Moreover, she is helping with some scale-up tests on CO_2 processing agents (CDPA). She analysed the CO_2 adsorption capacity of CDPA in a humid atmosphere with a light source (Figure 1.3).

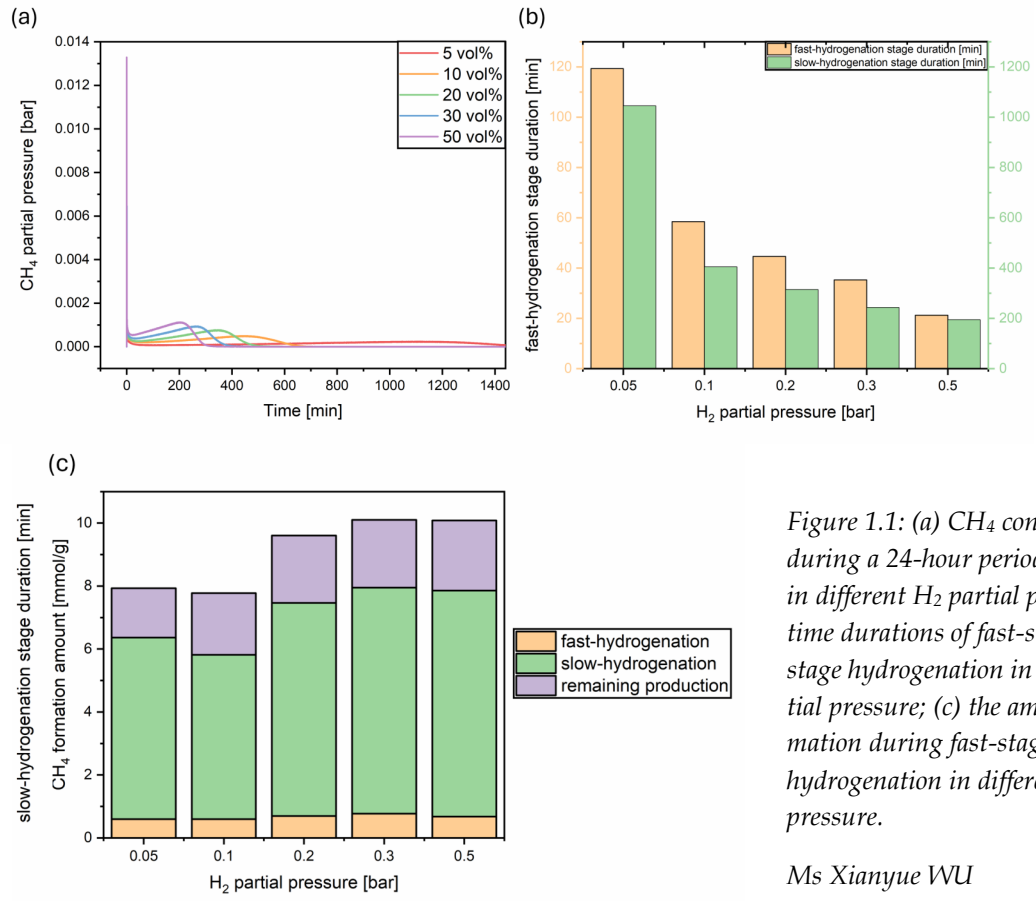


Figure 1.1: (a) CH_4 concentration change during a 24-hour period hydrogenation in different H_2 partial pressure; (b) the time durations of fast-stage and slow-stage hydrogenation in different H_2 partial pressure; (c) the amount of CH_4 formation during fast-stage and slow-stage hydrogenation in different H_2 partial pressure.

Ms Xianyue WU

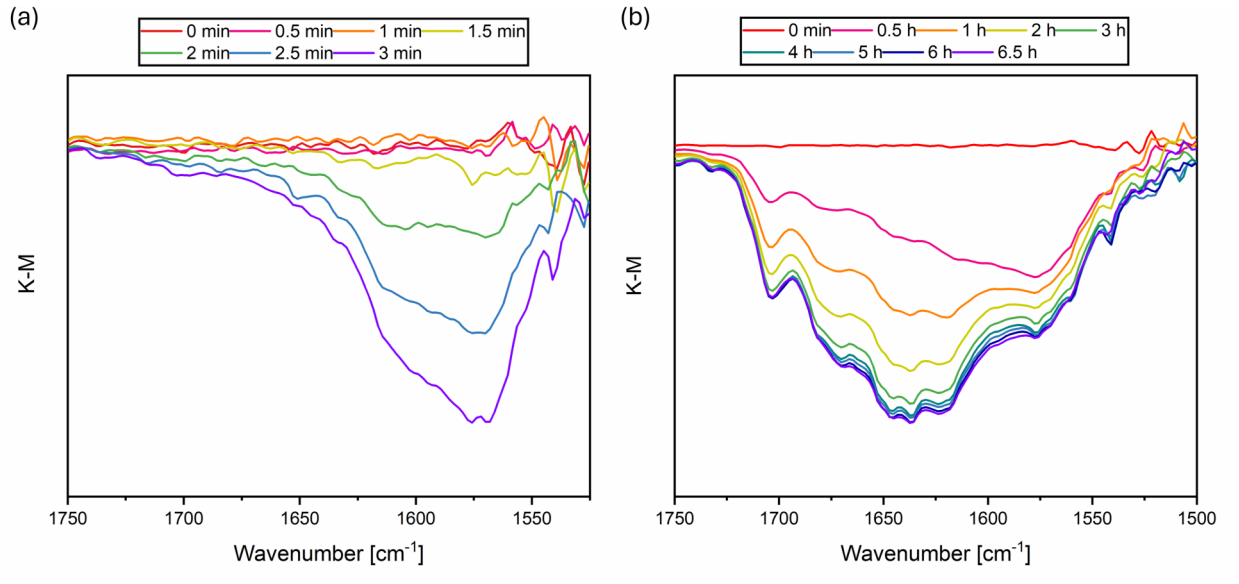


Figure 1.2: The differential in-situ DRIFT spectra of hydrogenation on Ni/$CaCO_3$ DFM in 20 vol% H_2/N_2 at 400 °C: (a) 0-3 min; (b) 0- 6.5 h.

Ms Xianyue WU

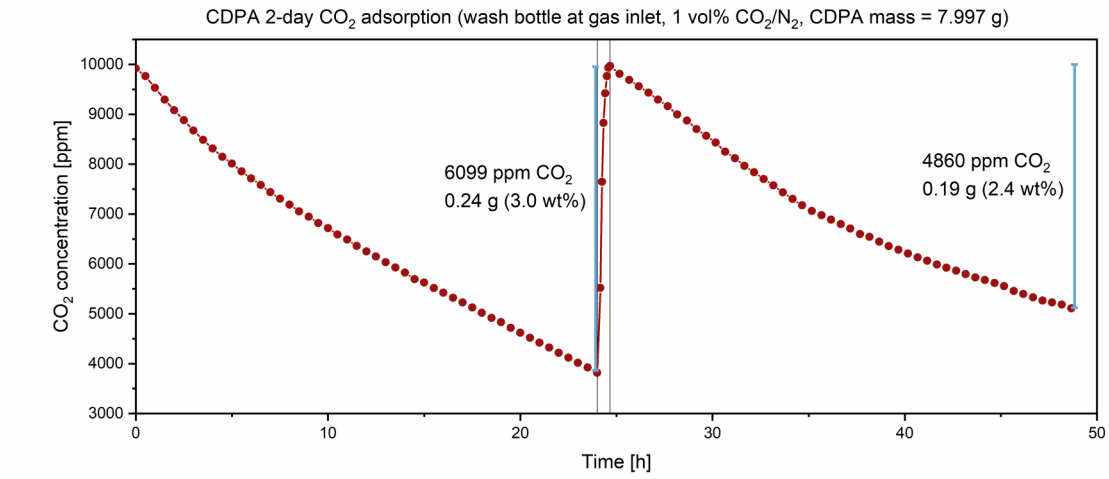


Figure 1.3: CO_2 concentration change for a 2-day CO_2 adsorption test on CDPA.

Ms Xianyue WU

Asst Prof Tej CHOKSI's (PI, NTU) group has contributed to the project along three fronts. A hypothesis-based approach to identify catalysts that can selectively transform CO_2 into CO, H_2, or higher-carbon number products was further refined. An active learning workflow was implemented to determine the minimum number of datapoints needed to build a pre-trained model. Reaction energies of CO_2 electro-reduction intermediates were capably predicted on Cu-Zn alloys using this active learning based approach. Trends in the thermodynamic driving forces for CO_2 electro-reduction to CO and HCOOH were computed, and these trends were used to rationalise experimentally measured faradaic efficiencies (collaborator: Prof Andrew WONG, NUS). This workflow will be publicly released with the corresponding publication.

Second, a set of scaling relationships (linear free energy relationships) to understand the selectivity of catalysts for the two-electron oxygen reduction were established. This work spans single- and dual-site catalysts comprising of earth abundant materials. A publication on this work has been prepared for submission.

Third, a computational framework to simulate reactions under ultrasound irradiation was further developed. This framework was used to understand how changing the gas phase environment (Ar:O_2 ratios) in ultrasound reactors impacts the selectivity of benzyl alcohol oxidation. Progressive increase in the O_2 fraction causes a proportional increase in fragmentation products like oxalic acid. These product distributions are explained using a mechanism-based microkinetic model.

CN10: Discovery and design of low-carbon routes to functional molecules

Prof Alexei LAPKIN (CAM)
Prof Ning YAN (NUS)

Guided by **Prof Alexei LAPKIN (PI, CAM)**, **Dr Zhen GUO (Senior Research Fellow, CARES)** has been working on the Computer-Aided Synthetic Planner (CASP) by implementing new features to the system. Newly added features include searching for similar molecules if the target molecule does not exist so that the retrosynthesis planning can be continued by targeting a similar molecule. Another feature is to search for reaction conditions given a desired chemical transformation. This feature is relevant to high-throughputs screenings and the design of experiments. It provides a range of reaction conditions (e.g., temperatures and pressures), as well as options of solvents and reagents.

A user can take this information obtained automatically as a starting point for experimental exploration. Dr Guo has also developed new machine learning algorithms for the prediction of molecular properties, mainly focusing on transferred learning and co-training. Next, Dr Guo will continue the update of CASP system targeting noise reduction of results and boosting search speed.

CN11: A database of bio-waste and bio-renewable feedstocks linked with chemical reactions prediction

Prof Alexei LAPKIN (CAM)

Mr Adarsh ARUN (PhD Student, CARES) commenced his PhD in January 2021, and focuses mainly on identifying sustainable routes from biowaste to value-added chemicals using networks and knowledge graphs (KGs). He is now finalising and completing case studies to simulate the exergetic performance of various pretreatment processes in the KG using open-source simulators such as Biosteam. At the same time, he is finalising and completing his thesis for submission.

Alongside this research, an internship project investigating the potential of LLMs (Large Language Models) in large-scale knowledge extraction for the biowaste to value-added chemicals domain has recently been concluded. This entailed the development of prompt engineering approaches to automatically extract entities and relationships relevant to the KG from unstructured text and has been included as a separate piece of work in the thesis.

ELECTROCHEMISTRY

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

Prof Adrian FISHER (CAM)
Prof Zhichuan XU (Jason) (NTU)
Assoc Prof Sui ZHANG (NUS)

Assoc Prof Sui ZHANG's (PI, NUS) group has continued to work on the electrochemical synthesis of microporous polymers, and has managed to publish a paper on the use of the membranes for carbon capture. They fabricated a series of carbazole-based conjugated microporous polymer (CMP) membranes with thicknesses of a few hundred nanometers through in-situ electropolymerisation for post-combustion carbon capture. Their findings reveal that various experimental conditions, including the monomer concentration, electric potential, and cyclic voltammetry (CV) cycling number, largely impact the polymerisation degree of the carbazole-based CMP, thus influencing the mode of polymer chain packing. An optimal polymerisation degree leads to a larger micropore size and a higher fractional free volume (FFV), thus allowing fast CO_2 transport. The study first demonstrates the feasibility of using CMPs to fabricate thin film composite (TFC) membranes for post-combustion carbon capture and confirms the high controllability of their micropores. These insights provide instructive guidance for the future advancement of CMP applications in membrane fabrication for gas separation and other fields which require precise micropore generation and design.

Our new portable electrolyser has now completed phase one trials and after some small modifications and will begin operation in Singapore.

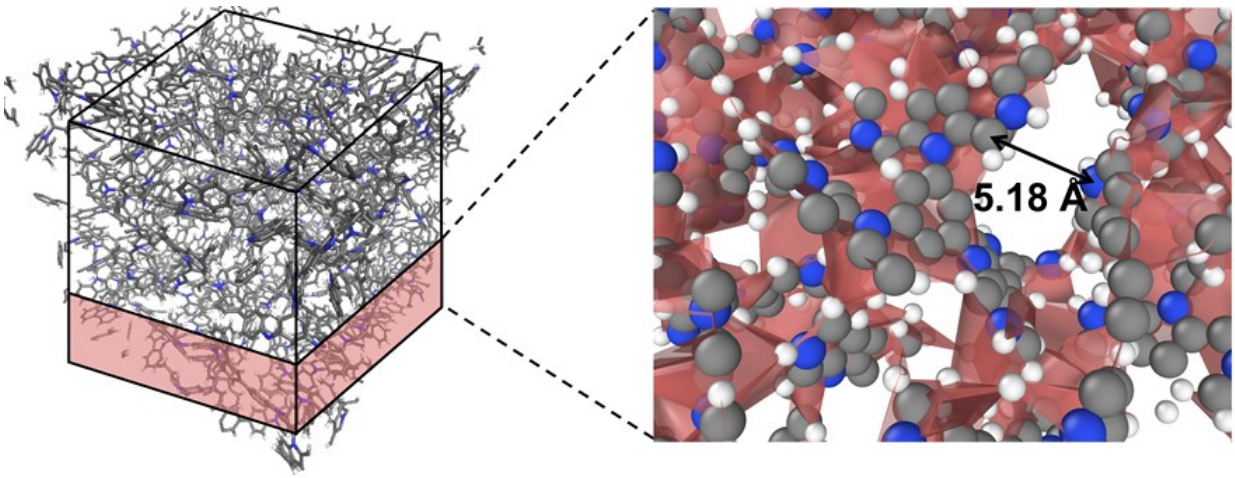


Figure 2.1: Simulated microscopic structure of CMP membranes.

Assoc Prof Sui ZHANG

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

Prof Adrian FISHER (CAM)

Prof Zhichuan XU (Jason) (NTU)

Dr Chencheng DAI (Research Fellow, NTU) has been investigating ammonia as a hydrogen carrier. One of the primary challenges lies in the processes of ammonia cracking. Traditional thermocatalytic ammonia cracking typically requires high temperatures and costly, sophisticated equipment, which limits its energy efficiency and applicability. The electrochemical ammonia cracking technique has been employed here to address these barriers. Pt-based catalysts are generally considered the most effective candidate for electrochemical ammonia oxidation reaction (AOR). However, they are also prone to suffer from catalyst poisoning by the AOR intermediates. In this study, we propose a method to mitigate these limitations. This process allows the in-situ cleaning of poisoning species using cathodic voltages and continuously enhances ammonia cracking by improving enhanced mass transfer through suppression of the diffusion layer thickness. Finally, an ultrastable current density of 1.95 A cm^{-2} is achieved with a faradaic efficiency (FE) towards hydrogen of 98.9 % over 1000 hours. These results surpass all current research on Pt-based ammonia electrocatalysis by orders of magnitude in terms of current density and durability time, demonstrating an ammonia e-cracker with high energy efficiency, stability, decentralisability, and scalability.

Additionally, ammonia production from electrochemical nitrate reduction by surface-reconstructed metal oxide catalyst ($LaCo_xSr_{2-x}O_4$ and $CoFe_xCr_{2-x}O_4$) has also been investigated. Enhancement in both the FE and activity towards ammonia generation were observed with optimised surface reconstruction. Moreover, a series of Pt-based catalysts were screened for electrochemical methanol oxidation reaction. Among them, $NdPt_3Fe$ shows the best performance, where the activity was improved, and the CO poisoning on catalyst surface was prohibited.

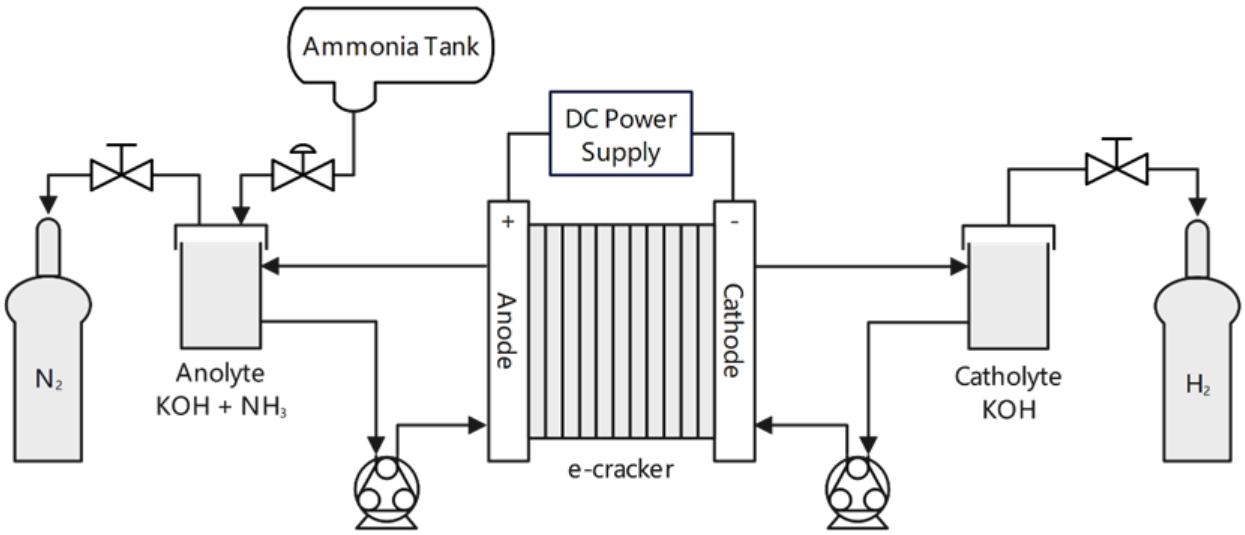


Figure 2.2: A schematic of an electrochemical ammonia cracker for hydrogen production.

Dr Chencheng DAI

CN8: Introducing new hydrogen-rich town gas to the residential and commercial cooking sectors

Prof Markus KRAFT (CAM)
Assoc Prof Wenming YANG (NUS)

The project aims to identify the combustion properties associated with the use of new hydrogen-rich town gas in residential and commercial cooking sectors. The primary focus areas are the development of standardised methods for hydrogen (H_2) combustion diagnostics and the study of emissions from various gas compositions and stove types.

During this reporting period, the team designed the experimental setup for new hydrogen-rich town gas combustion utilising two workflows: (a) a non-premixed burner equipped with a laser diagnostics system for in-flame species detection, and (b) residential and commercial stoves paired with a gas analyser for emission measurement. In workflow (a), the experiments are designed to investigate H_2 blending in natural gas pipelines, which may contribute to reducing terminal pollutant emissions.

The team conducted experiments using a custom-built non-premixed burner equipped with laser diagnostics. A pure methane (CH_4) flame was selected as the baseline, and varying percentages of H_2, ranging from 0% to 15%, were added to the flame. Both soot tendency and nitric oxide (NO) radicals were measured using laser-induced incandescence (LII) and laser-induced fluorescence (LIF) techniques. As the H_2 content increased from 0% to 15%, a clear reduction in soot formation was observed, attributed to the replacement of CH_4 with H_2, a carbon-free fuel. However, the variation in NO emissions across different flames was minimal, likely due to the slight increase in combustion temperature being offset by significant heat loss from H_2 addition, thereby balancing out the potential for increased NO formation.

For workflow (b), the experiment was designed based on the existing town gas used in Singapore, which already contains a high proportion of H_2, approximately 50% by volume. In collaboration with engineers from City Energy, the team proposed three different town gas-like mixtures with varying compositions to represent potential scenarios of incorporating green H_2 into existing town gas production. The compositions of these gas mixtures were calculated, considering both the Calorific Value and Wobbe Index. For this experiment, City Energy provided both residential and commercial stoves for testing. The residential stove is the latest model from Rinnai, commonly used in Singaporean households, featuring battery-powered spark ignition. The commercial stove is a multi-nozzle model typically used in food courts and hawker centers, characterised by strong power output, large size, a multi-layer nozzle design, and a pilot flame for ignition.

Given the high H_2 content in the existing town gas and the proposed gas mixtures, the team conducted comprehensive risk assessments covering four main areas: storage of the town gas and gas mixtures, setup of the experimental cooking stoves and emission measurement system, flame handling and emission measurement, and flame shut-off procedures. To ensure safety, all experiments will be conducted within fume hoods, with gases stored in a separate gas cylinder room. Connections will be made using stainless steel tubing, and thorough leak tests will be performed prior to conducting any experiments. These precautions are essential due to the unique properties of hydrogen-rich gas mixtures.

Figure 3.1: Cooking stoves used in the experiment. Left: Residential stove commonly used in households in Singapore. Right: Commercial stove typically used in food courts and hawker centers in Singapore.

CN12: Dehydrogenation of alternative liquid organic hydrogen carriers (LOHC)

Prof Markus KRAFT (CAM)
Prof Rong XU (NTU)

This project aims to develop scalable flame synthesis of novel and affordable catalysts for the dehydrogenation of perhydro-dibenzyltoluene (H18-DBT) and other alternative liquid organic hydrogen carriers (LOHCs) to diversify supplies and reduce the cost of imported hydrogen (H_2).

LOHCs are chemical compounds that can absorb and release H_2 through a chemical reaction and are potential vectors for H_2 storage and transportation. H18-DBT is a promising LOHC due to its high H_2 density (6.21 wt%), liquid phase at room temperature, and low toxicity. In this project, the team synthesised platinum (Pt) / titanium dioxide (TiO_2) catalysts using flame-synthesised TiO_2 nanoparticles as a support and investigated its performance in the dehydrogenation of H18-DBT.

During this reporting period, the team tested catalysts with different Pt precursors, varying Pt loading amounts, and sulphur (S) loading amounts. A 0.5 wt% Pt loading was found to achieve a high degree of dehydrogenation (DoD). This specific loading, when combined with the Tetraammineplatinum(II) nitrate ($[Pt(NH_3)_4](NO_3)_2$) precursor, exhibited the highest DoD of approximately 94% after 6 hours of dehydrogenation, as illustrated by the pink line in Figure 3.2.

The team further investigated doping the best performing Pt/TiO_2 catalyst (0.5 wt% Pt/TiO_2, $[Pt(NH_3)_4](NO_3)_2$ Pt precursor, commercial TiO_2 support) with different S precursors. The following S precursors were tested: ammonium sulphate ($(NH_4)_2SO_4$), thiourea ($SC(NH_2)_2$), 2-mercaptoethanol (2-ME) and 2-mercapto-5-nitrobenzimidazole (MNB). As shown in Figure 3.3, the addition of 2-ME was found to enhance dehydrogenation, with an optimal S loading amount of 0.15 wt%. Further increases in S loading (beyond 0.3 wt%) did not significantly impact dehydrogenation..

Figure 3.4 presents the hydrogen temperature-programmed reduction (H_2-TPR) characterisation results. It is observed that peaks appear at approximately 300°C in the samples doped with S (Figures 3.4(b) and (d)), suggesting that S doping enhances reducibility. Additionally, the peak in Figure 3.4(d) is higher than that in Figure 3.4(b), suggesting the presence of strong metal-support interactions between the Pt particles and the TiO_2 support.

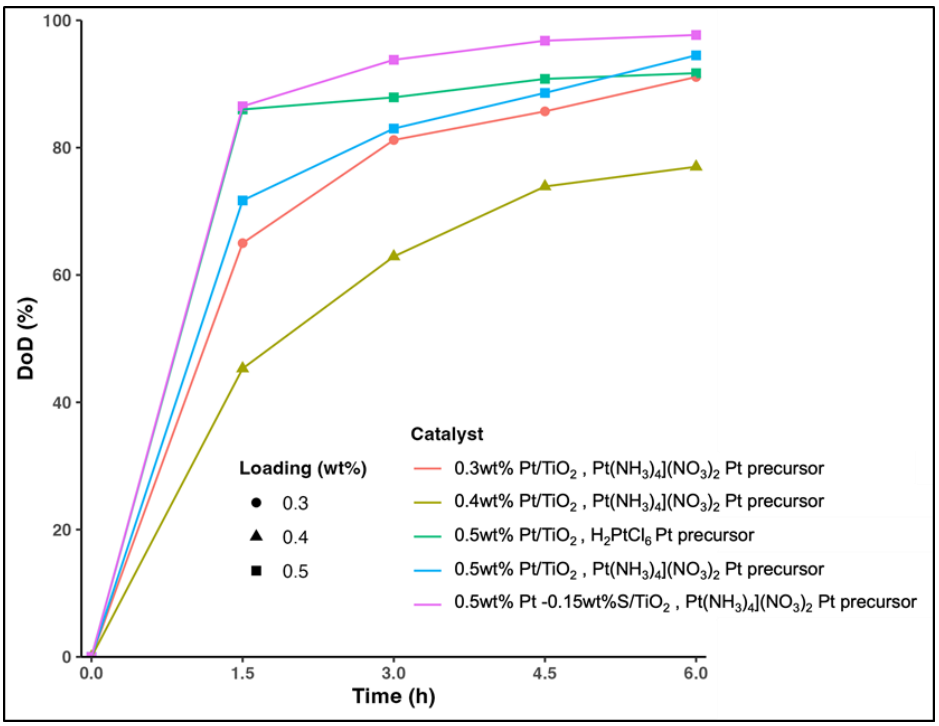


Figure 3.2: Degree of dehydrogenation (DoD) performance over 6 hours across catalysts with different Pt wt% loadings and Pt precursors.

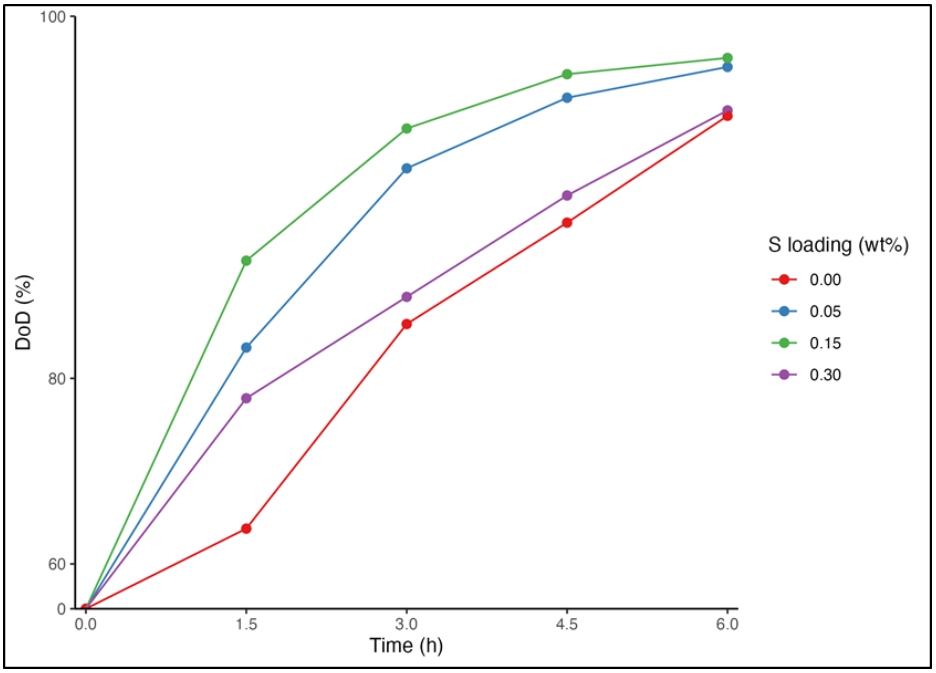


Figure 3.3: Degree of dehydrogenation (DoD) performance over 6 hours across different 2-ME loadings on 0.5 wt% Pt/TiO_2 catalysts.

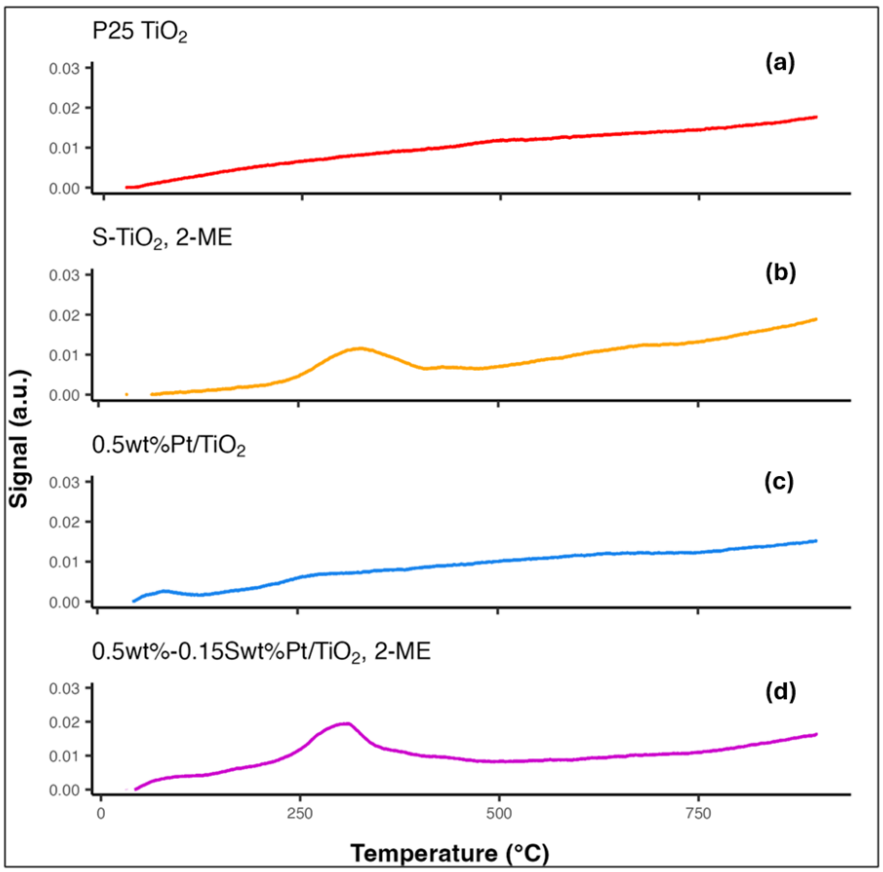


Figure 3.4: Hydrogen-Temperature-Programmed Reduction (H_2-TPR) characterisation results of catalyst samples.

CN13: Conversion of CO_2 to useful chemicals

Prof Markus KRAFT (CAM)
Prof Rong XU (NTU)

The project aims to explore solutions to the underlying issues behind the failure of electrochemical carbon dioxide (CO_2) reduction cells observed in previous studies (mainly attributed to the flooding of gas diffusion electrodes (GDEs)), and to investigate the scale-up of the reduction cells.

During this reporting period, the team continued the development and testing of new GDE designs that can mitigate the flooding issue caused by the loss of hydrophobicity during the CO_2 reduction reaction (CO_2RR). The new GDE was fabricated by depositing a 50 nm thick copper (Cu) layer onto a polytetrafluoroethylene (PTFE) membrane with an average pore size of 0.22 µm, known for its robustness and excellent hydrophobic properties. The deposition was performed using an electron beam evaporation system at a controlled evaporation rate of 0.2 Å/s, with precise monitoring of the film thickness. Following the Cu coating, the PTFE membrane was mounted onto a platinum electrode clip to serve as the working electrode. A Cu mesh was used as the counter electrode, and sodium hydroxide (NaOH) was employed as the electrolyte. Electrochemical oxidation was conducted on the Cu-coated PTFE membrane at a constant current density, with anodisation times ranging from 1 to 3 hours.

Systematic experiments were conducted to evaluate the performance of these electrodes under different anodisation durations for CO_2 reduction. The electrode anodised for 1 hour exhibited

a promising Faradaic Efficiency (FE) of 31.2% for ethylene (C_2H_4) and 51.9% for total C_2+ products. Increasing the anodisation duration to 2 hours enhanced the performance, with the FE of C_2H_4 rising to 33.2% and the FE of total C_2+ products increasing to 57.9%. However, further extending the anodisation time to 3 hours negatively impacted the performance, reducing the FE of C_2H_4 to 16.5% and significantly lowering the FE of total C_2+ products to 26.3%. During this period, the FE of hydrogen (H_2) increased to 21.4%, as illustrated in Figure 3.5.

The stability of the electrode anodised for 2 hours was tested under operational conditions of 200 mA cm^{-2} in a flow-cell electrolyser. This electrode retained 78% of its initial FE of C_2H_4 after 12 hours of continuous operation (Figure 3.6).

To further investigate the impact of Cu layer thickness, additional experiments were conducted using PTFE membranes coated with Cu layers of 25 nm, 50 nm, and 100 nm thicknesses, each subjected to identical 2-hour anodisation conditions. As shown in Figure 3.7, the FE of C_2H_4 and total C_2+ products decreased when the Cu layer thickness deviated from the optimal 50 nm, highlighting the significance of Cu layer thickness in determining the electrode's performance for CO_2 reduction.

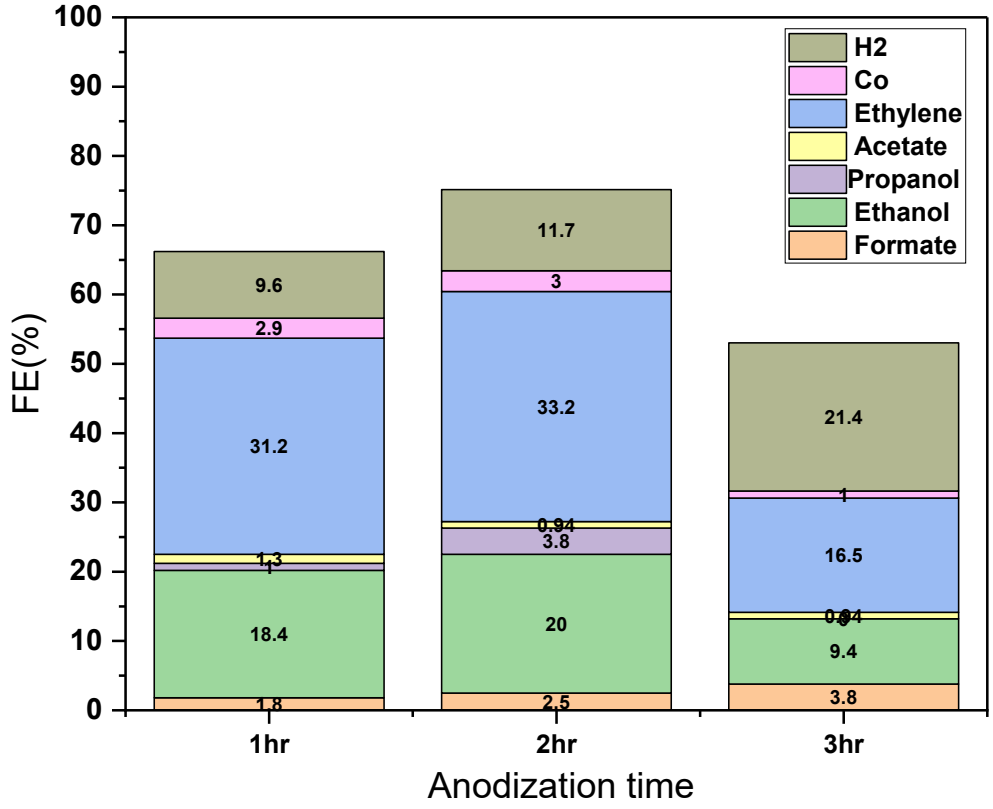


Figure 3.5: Faradaic efficiencies (FEs) for hydrogen (H_2), carbon monoxide (CO), ethylene (C_2H_4), acetate (C_2H_3O), propanol (C_3H_8O), ethanol (C_2H_6O) and formate (CH_2O_2) in the CO_2 reduction reaction (CO_2RR) across various experimental sample electrodes subjected to different anodisation durations in a flow cell.

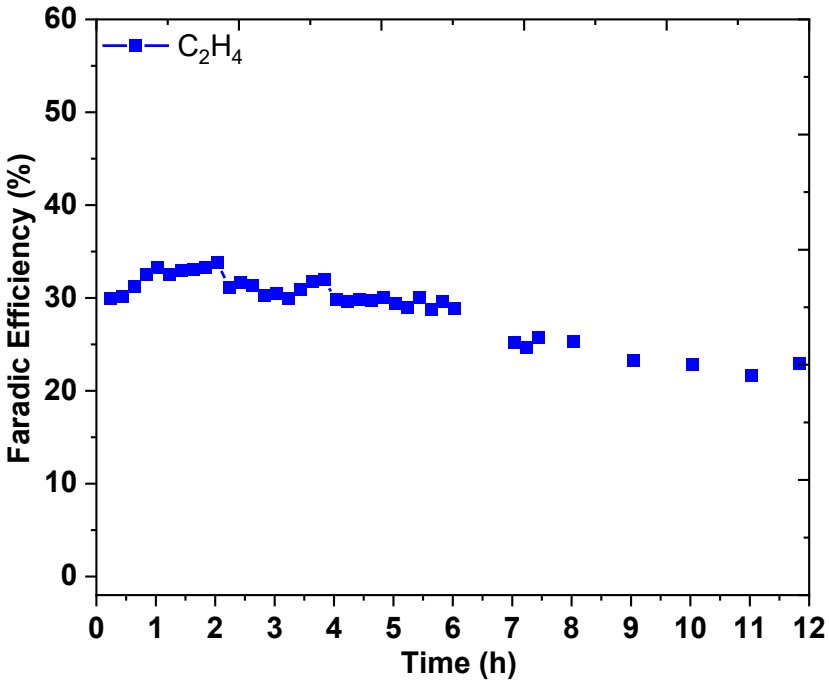


Figure 3.6: Faradaic efficiency (FE) of ethylene (C_2H_4) in a flow-cell electrolyser.

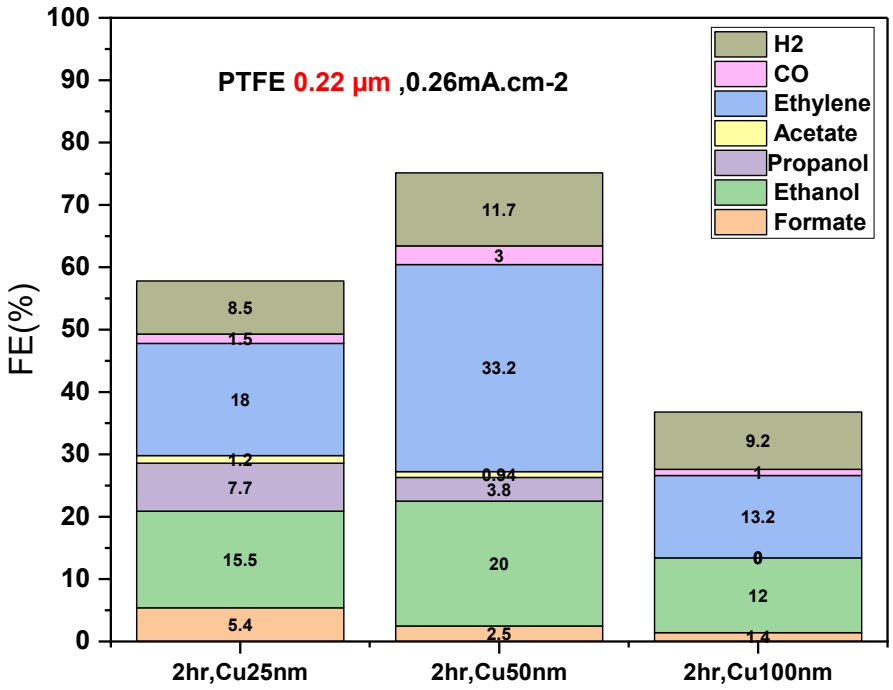


Figure 3.7: Faradaic efficiencies (FEs) for hydrogen (H_2), carbon monoxide (CO), ethylene (C_2H_4), acetate (C_2H_3O), propanol (C_3H_8O), ethanol (C_2H_6O) and formate (CH_2O_2) in the CO_2 reduction reaction (CO_2RR) across various experimental sample electrodes with different Copper (Cu) layer thicknesses in a flow cell.

MARITIME DECABONISATION

CN1: Air pollutant measurements with aerial devices

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

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

During this reporting period, the team continued its collaboration with the Maritime & Port Authority of Singapore (MPA) to plan a potential trial utilising a UAV for ammonia leak detection during ammonia bunkering activities. Additionally, the team explored the possibility of differentiating emissions generated by shipping activities from those generated by other sources. A literature review was conducted to identify suitable sensors for installation on the UAV, leading to the selection of a compact, real-time, wearable 5-wavelength Ultraviolet-Infrared Black Carbon monitor (MA200, AethLabs, San Francisco, CA, USA). The MA200 sensor is capable of distinguishing between Brown Carbon (BrC) and Black Carbon (BC) based on their light-absorbing properties. While BC is typically associated with most carbon-containing combustion emissions, such as those from traffic and industry, BrC is primarily linked to biomass combustion and shipping emissions, and acts as a significant climate forcer. Utilising the MA200 sensor in conjunction with the UAV provided unique insights into the three-dimensional dispersion of emissions.

The team obtained UAV operating permits from the Civil Aviation Authority of Singapore (CAAS) for two locations: Marina Bay Sands (MBS), which has direct exposure to shipping emissions, and University Town Green (UT), which has minimal direct exposure to shipping emissions. Several measurement campaigns were conducted at both sites, and the data obtained were processed and analysed.

Figure 4.1 shows the two measurement sites, indicated by red stars at Marina Bay Sands (MBS) and University Town Green (UT). Measurement dates were carefully selected to ensure that the UT site was not significantly influenced by sea breeze, which can carry significant shipping emissions inland through atmospheric dispersion. Similarly, measurements at the MBS site were conducted when winds were primarily blowing from the south or southeast, to ensure that shipping emissions were directed towards the site. Figure 4.2 displays the ship traffic data obtained from MarineTraffic (a community-driven project based on research collaboration), near Singapore on one of the measurement dates (14 July 2024), highlighting the potential for greater impact of shipping emissions on the MBS site and the east coast of Singapore compared to the UT site or other inland regions of Singapore. Note that the results obtained are limited due to restrictions on permitted flight dates and prevailing weather conditions.

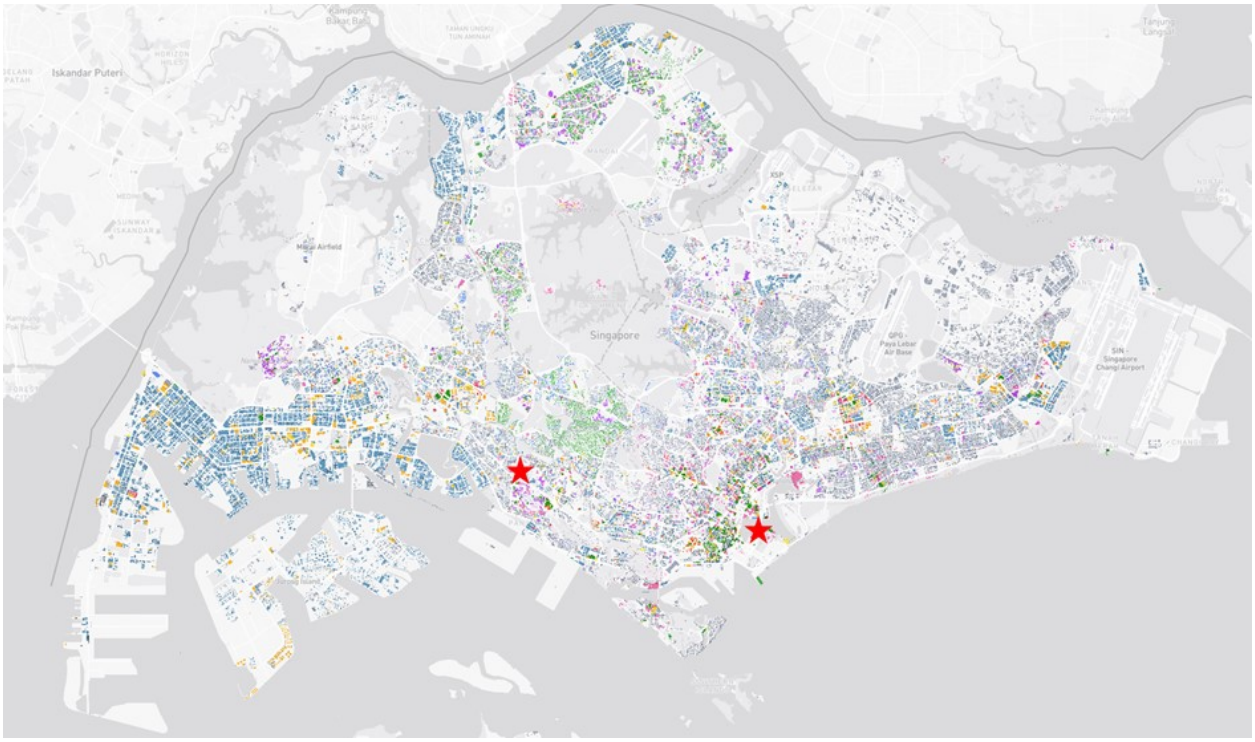


Figure 4.1 Measurement sites indicated by red stars at Marina Bay Sands (MBS) and University Town Green (UT).

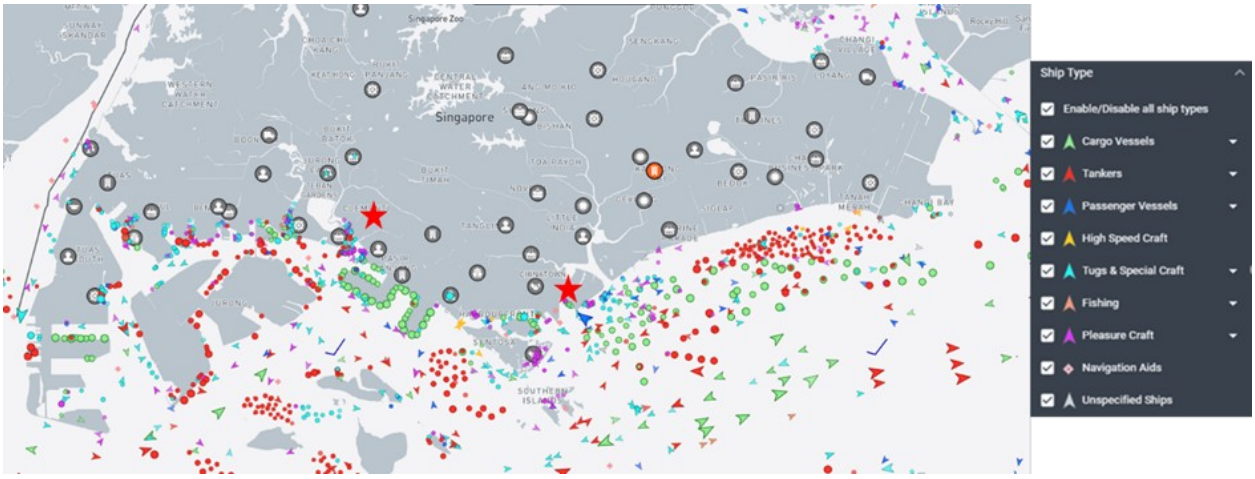


Figure 4.2: Ship traffic data obtained from MarineTraffic near Singapore on 14 July 2024. Ship types are indicated by their colour and shape. The chosen measurement sites of Marina Bay Sands (MBS) and University Town Green (UT) are marked by red stars.

Figure 4.3 illustrates the concentration of Equivalent Black Carbon (eBC) at various heights. The term eBC refers to BC measured by the light absorption method. Distinct vertical profiles of eBC concentrations were observed at the same location on different days, suggesting that wind patterns and particulate matter composition are likely dominant factors influencing the concentration profile. The results indicate that pollutant dispersion can vary up to a height of 150 meters. Given that some residential buildings in Singapore exceed 150 meters, these findings suggest the potential for tiered pollutant exposure for residents living at different elevations. Further measurements of various pollutant species are needed to test this hypothesis.

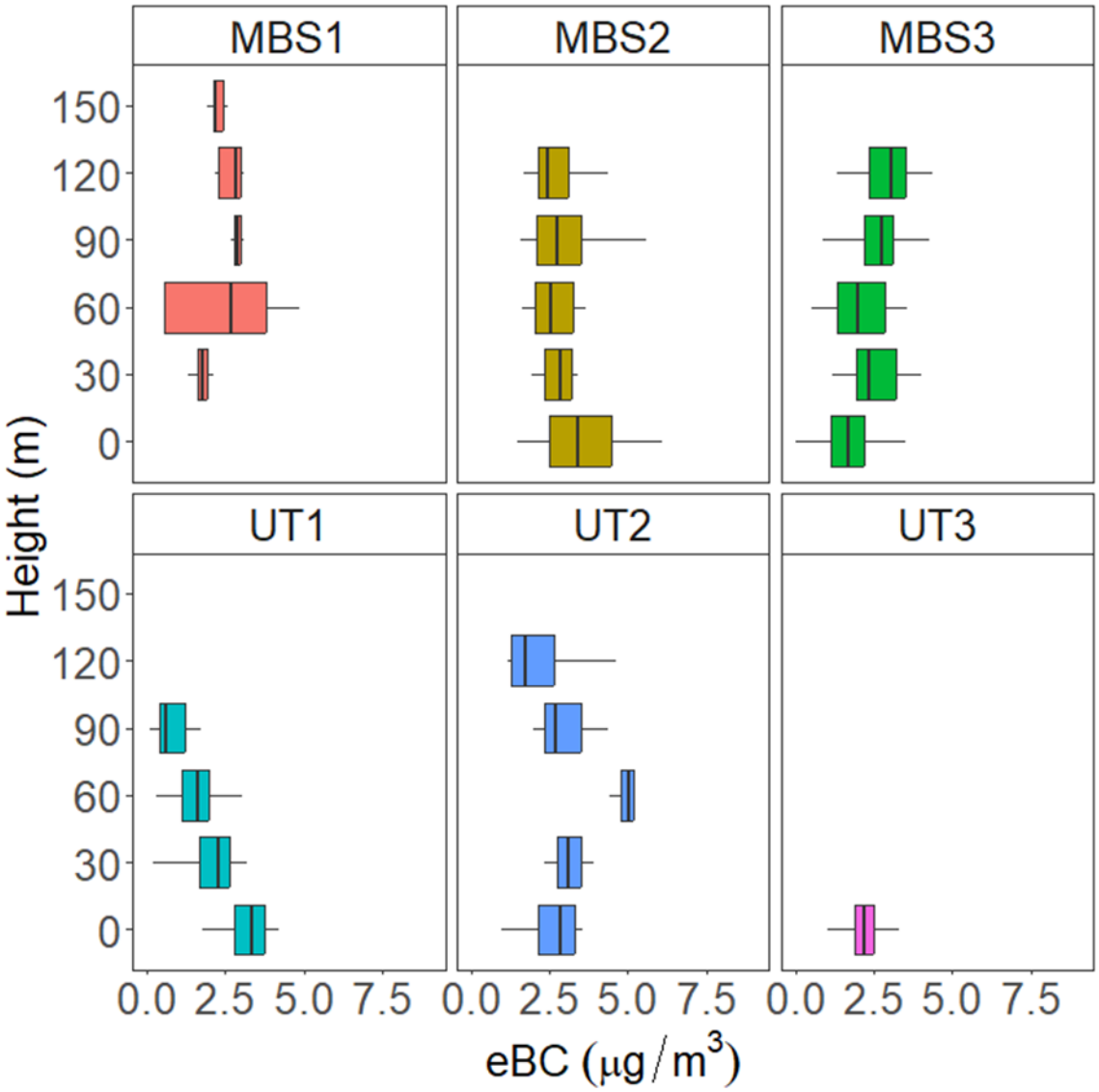


Figure 4.3: Box plots showing the concentrations of Equivalent Black Carbon (eBC) across various heights at the Marina Bay Sands (MBS) and University Town Green (UT) sites. The datasets are grouped by the measurement site and date (e.g., MBS1 represents the first measurement conducted at the MBS site).

Figure 4.4 shows the Absorption Ångström Exponent (AAE) parameter measured at the MBS site. An elevated AAE (i.e., AAE>1.2) suggests the influence of BrC, which could originate from shipping emissions and/or biomass combustion. Data from the Fire Information for Resource Management System indicate regional biomass combustion activities during all measurement dates. Consequently, the current measurement data are insufficient to conclude that the observed elevated AAE is solely attributable to shipping emissions. Further measurements and detailed analysis are required to distinguish between emissions from shipping activities and other sources.

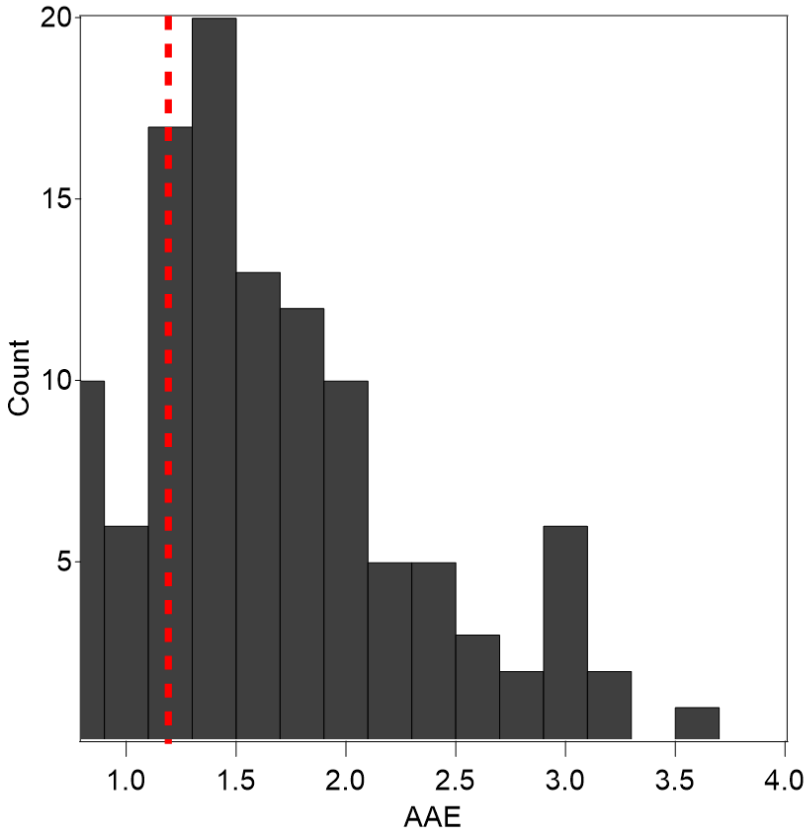


Figure 4.4: The Absorption Ångström Exponent (AAE) parameter of measured particles. The red line indicates the AAE of Black Carbon (BC) without Brown Carbon (BrC) influence during previous measurements in Singapore.

Dr Mutian MA (Research Fellow, CARES) has improved the drone sampling platform design to reduce drone downwash impact on particulate matter concentration. BC and brown carbon BrC were identified as two main constituents to identify for 1) vertical distributions of concentration of pollutants near port regions that could lead to tiered exposures for residents living at various heights (i.e., ground level versus up to 250m).

Dr Ma took BC and BrC ambient measurements using the drone platform from (site 1) University Town (UT) in the National University of Singapore and (site 2) Marina Boulevard at a site <1km from ships near Marina Bay Sands. Several measurements were taken on separate days due to limited time windows granted by CAAS. Figure 4.5 shows the drone sampling platform at the MBS site and ships near the sampling location. Figures 4.3 and 4.4 show the preliminary results of the characteristics of BC and BrC (reported via the absorption Ångström exponent (AAE)). No consistent vertical trend of particle concentration was observed suggesting multiple measurements for pollutants are needed for public health interests (e.g., 50m, 100m, 150m, 200m and 250m for residential buildings). A larger absorption contribution by BrC at the MBS site suggested potential influence by ship emission. Note that ships may emit different types of organic aerosol (i.e., BrC is part of organic aerosol) with elevated toxicity and this requires further investigation.

The results have sufficient novelty to be the foundation for a research article with additional measurements and analysis planned. The preliminary work was awarded an oral presentation at the 16th International Commission on Atmospheric Chemistry and Global Pollution/18th International Global Atmospheric Chemistry.

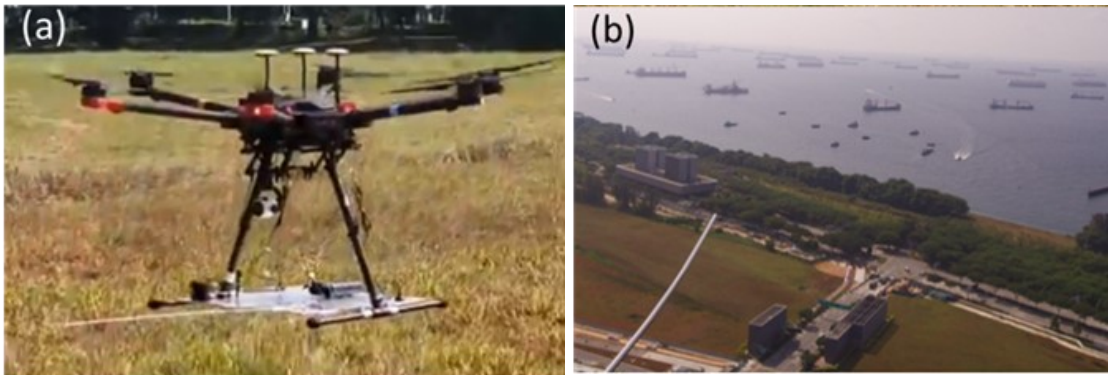


Figure 4.5: (a) CARES drone sampling platform (DJI m600 pro with MicroAeth MA200 sampler) and (b) ships near the port region when the drone was hovering and taking measurements.

Dr Mutian MA

Dr Yong XU (Research Fellow, CARES) has been conducting Numerical Simulation of Diesel-Methanol Combustion in a Constant Volume Chamber under the guidance of **Prof Epaminondas MASTORAKOS (PI, CAM)**. Dr Xu found that most experimental studies focused on engine performance and engine-out emissions. However, the autoignition and flame propagation inside the combustion chamber were not well understood.

Dr Xu focused on the non-premixed combustion in a constant volume chamber. This project follows two steps: initially, he is simulating 0D Diesel-Methanol Combustion (DCMC), where xi1 represents Diesel (modelled as *n*Heptane) and xi2 Methanol, with xi=0 indicating air. The DCMC equation is derived for the two conditioning variables, mixture fraction and reaction progress variable. The numerical results from 0D-DCMC will describe the basic structure of the autoignition and subsequent flame propagation in mixture fraction space. He has started investigating the influence of initial temperature and pressure (in the combustion chamber) on the automation and flame propagation of dual-fuel mixtures. As tabulated in Table 1, the initial temperature includes 700K, 800K, and 1000K. The initial pressure spans from 5 bar to 30 bar.

It has been shown that autoignition can occur in some scenarios. However, due to the use of a flawed reaction mechanism, only initial simulation results were obtained. Therefore, a better mechanism is being sought for the in-house code.

Subsequently, Dr Xu is running CONVERGE simulations for 3D constant volume combustion. These include native CONVERGE without any turbulent combustion model (other than the correct chemistry) or with LES. The case setup includes gas simulation, parcel simulation, combustion modelling, and turbulence modelling using Adaptive Mesh Refinement (AMR) technology. They aim to clarify the generation and evolution of autoignition and the propagation of the dual-fuel flame.

Table 1: Initial test conditions in the combustion chamber

P/bar	Tair/K			Tfuel/K
5	700	800	1000	300
10	700	800	1000	300
20	700	800	1000	300
30	700	800	1000	300

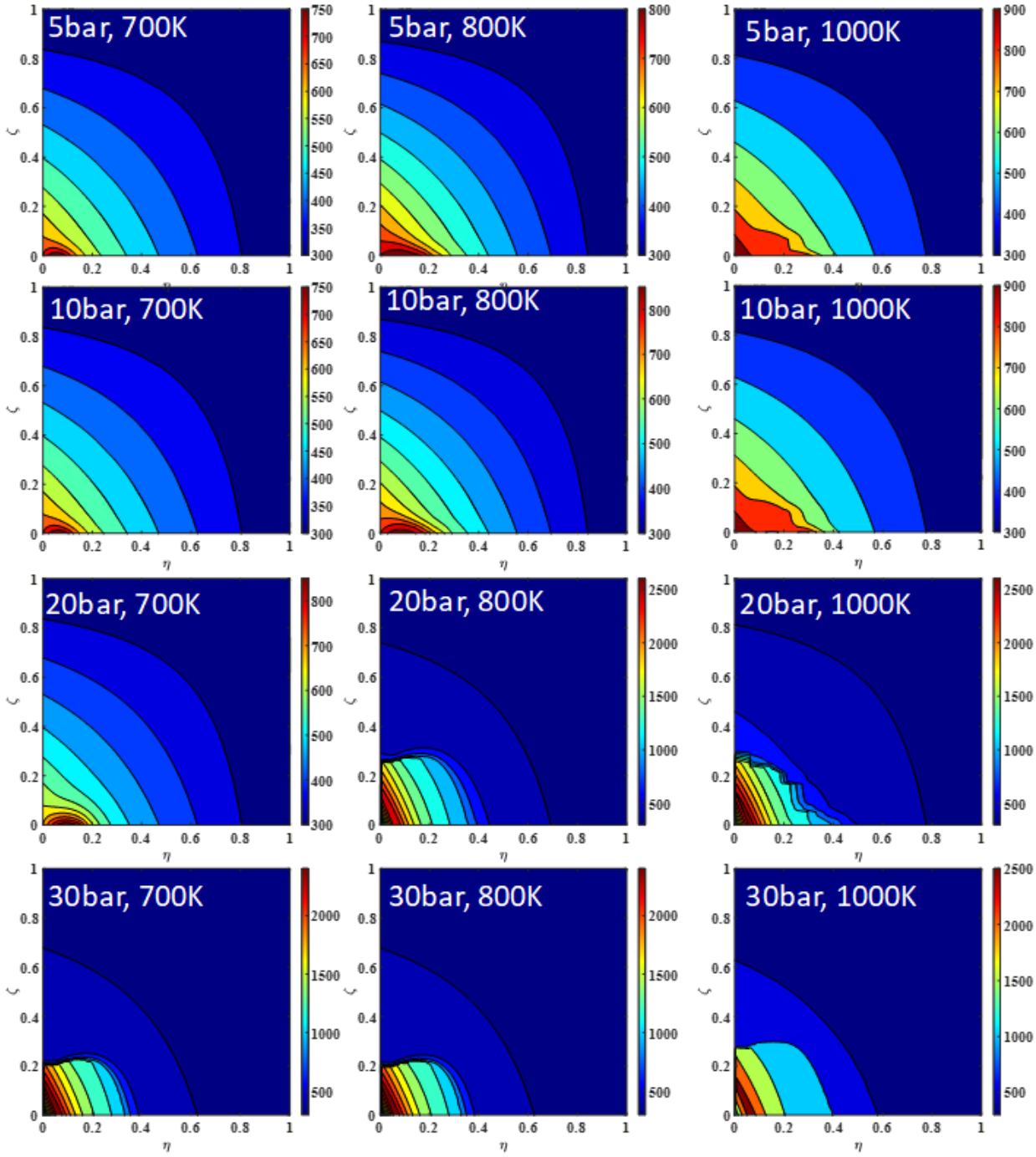


Figure 4.6: 0D dual-fuel combustion simulation. The plots present the influence of initial air temperature and chamber pressure on the autoignition of dual-fuel mixtures, coloured by temperature (colour bar: gas temperature [K]). The horizontal and vertical symbols, η and ζ, indicate the mass fractions of CH_3OH and n-C7H16, respectively.

Dr Yong XU

CN3: Lifecycle and system-level studies of marine decarbonisation

Prof Epaminondas MASTORAKOS (CAM)

Dr Li Chin LAW (Research Fellow, CARES) has been showcasing the CII and Fuel EU Maritime calculator (https://emi-cast.com) and the low-carbon ship calculators (https://lowcarbonship.com) at several exhibitions this reporting period, raising awareness among maritime stakeholders about the importance of shipping decarbonisation. The demonstration also provided insights into the alternative options of low-carbon pathways. Currently, the focus is on analysing historical data from a vessel provided by Laskaridis Shipping Co. Ltd. An NDA was signed with Laskaridis Shipping and METIS in the previous reporting period to share data to input into CARES' modelling tools.

By understanding the vessel's operational profile and voyage patterns, Dr Law aims to model real ships powered by various alternative fuels. This modelling will integrate ship data with a lifecycle assessment (LCA) database to evaluate the effectiveness of different low-carbon solutions, such as ammonia, methanol, and onboard carbon capture, in reducing emissions. This research is expected to provide a realistic assessment of the effectiveness of various decarbonisation options.

In addition, the behaviour of the vessel during its voyages and the impact of environmental conditions will be factored into the analysis.

The spin-off by Dr Law, EMICAST, is currently conducting a feasibility study on carbon capture onboard an LNG carrier, focusing on the techno-economic analysis and economic modelling of an LNG carrier equipped with an OCCS (Onboard Carbon Capture System). Additionally, EMICAST plans to develop a big data processing tool to visualise a ship's operational profile and emission rates based on the complex historical data. By integrating AI expertise with scientific and naval knowledge, this tool will enable the generation of CII reports and the evaluation of various low-carbon solutions, allowing for the selection of the most cost-efficient option.

The workflow of the AI-based low-carbon analyser is divided into three phases as summarised in Figure 4.7. The product is currently in its first phase of development, Data Processor & Analyser Development. This phase requires advanced coding for high-volume data ingestion, preprocessing, and transformation, as well as the implementation of machine learning algorithms for accurate predictive modelling. Successful completion of this phase is crucial before advancing to the next stages of development.

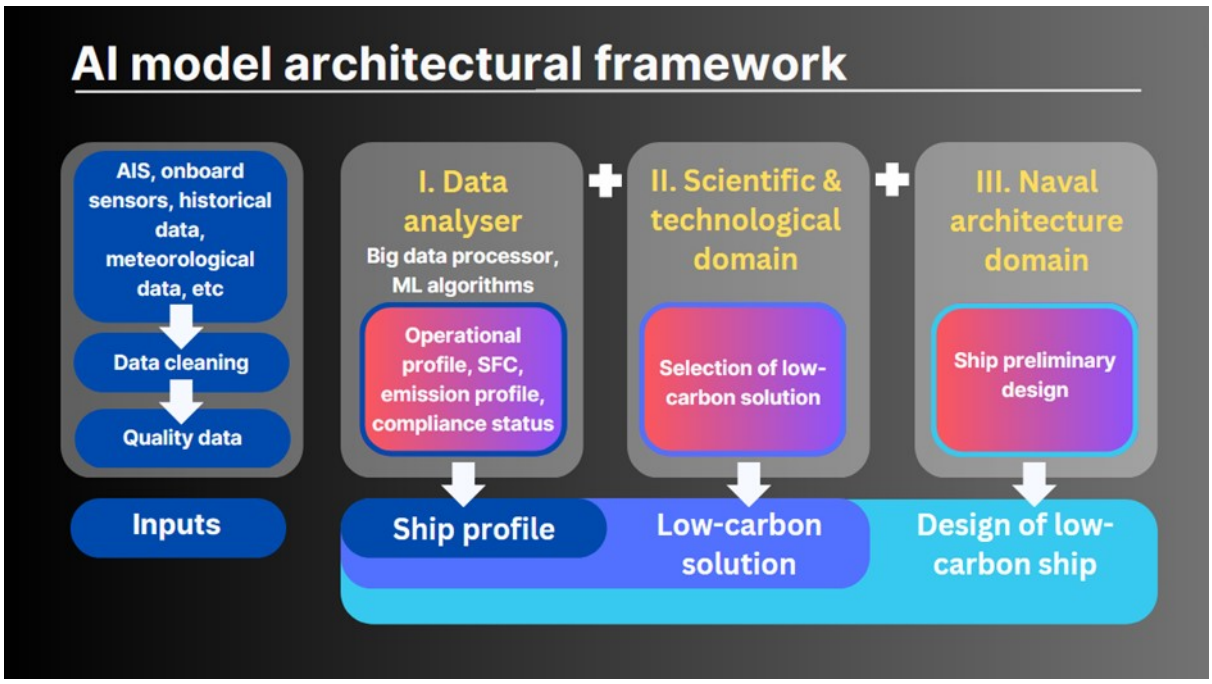


Figure 4.7: The AI-based ship design analyser consists of three core components. The first component is the data analyser, which acts as the central engine, processing large volumes of complex input data and transforming them into interpretable graphical outputs. These outputs are then passed through the scientific and technological domains, where the system autonomously evaluates the ship's performance with various low-carbon solutions. The system identifies the most effective low-carbon option tailored to the ship's specific design. In the third phase, naval architecture expertise is utilised, facilitating the design of a low-carbon ship based on the selected solution.

Dr Li Chin LAW

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

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

Dr Yangyang LIU (Research Fellow, CARES) has been investigating ammonia as a promising alternative for marine fuel. However, accidental leakage of ammonia can pose a risk such as fatalities, injuries, financial losses, and environmental damage, highlighting the significance of safety regulations for any ammonia application. Traditional consequence assessments for hazardous material releases focus on the mean concentration to determine exposure or lethal zones. Dispersion models and Computational Fluid Dynamics (CFD) simulations are common methods to estimate this mean concentration. However, these assessments are only in terms of the mean value of the ammonia neglect concentration fluctuations, potentially exposing personnel to unsafe levels even within seemingly safe zones.

To address this gap, under the guidance of **Prof Epaminondas MASTORAKOS (PI, CAM)**, Dr Liu conducted a study that goes beyond the mean approach. In this study, a probabilistic approach based on the presumed probability density function (PDF) was used to analyse the instantaneous concentration of ammonia leaked during ship-to-ship bunkering, a vital maritime activity. CFD simulations were used to calculate the mean concentration and quantify the variance of concentration fluctuations. Unlike traditional methods that rely solely on the mean concentration, this approach assesses the probability of ammonia con-

centrations exceeding established threshold limits. Results show significantly larger areas with a 1% or 10% chance of exceeding threshold concentrations compared to assessments based solely on the mean concentration. In simpler terms, personnel can still be exposed to dangerous levels even in areas deemed safe by traditional mean-only methods. Therefore, incorporating concentration fluctuations into consequence assessments and safety regulations is essential for ensuring safer ammonia bunkering operations. The proposed probabilistic approach using the PDF offers a more informative framework for quantitative risk assessment.

Figure 4.8 illustrates three regions where: the mean ammonia mass fraction exceeds 2.2×10^{-4}, i.e., $Y_m \geq 2.2\times10^{-4}$; the probability of ammonia mass fraction surpassing 2.2×10^{-4} is greater than 0.01, i.e., $F(Y_m \geq 2.2\times10^{-4}) \geq 0.01$; and the probability of ammonia mass fraction exceeding 2.2×10^{-4} is greater than 0.1, i.e., $F(Y_m \geq 2.2\times10^{-4}) \geq 0.1$. The figure compares these regions in terms of plume morphology (width, height, and length) from the X-Z perspective. Notably, the exposure regions determined by the probabilistic approach with chances of 0.01 and 0.1 are larger than those identified solely by the mean mass fraction. This observation underscores the significant impact of fluctuations of the mass fraction on risk zone delineation, highlighting the inherent uncertainty in relying solely on mean values.

This work has been consolidated into a research paper and is currently under review by the co-authors.

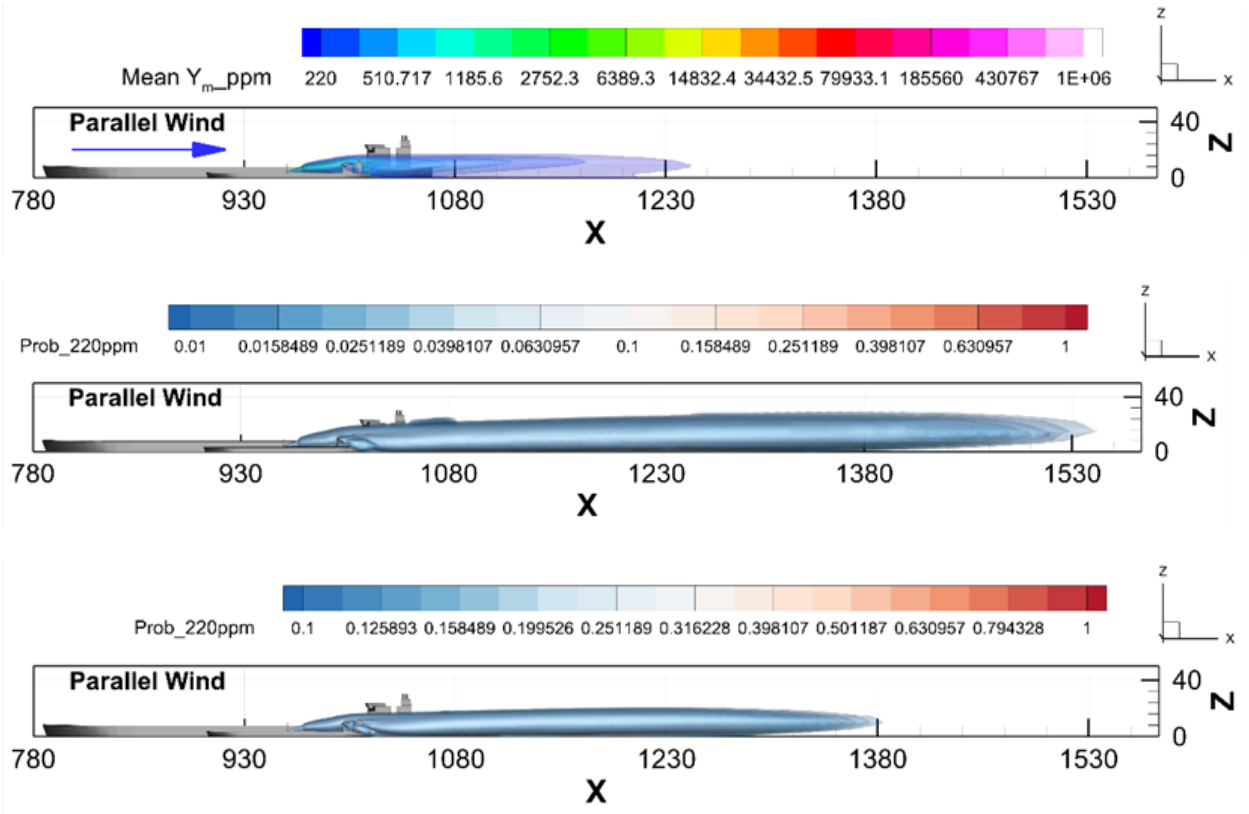


Figure 4.8: X-Z plane projection of risk zones for ammonia leakage in the parallel wind case: (top) regions with mean mass fraction exceeding 2.2×10^{-4}; (middle) regions where the probability of ammonia mass fraction surpassing 2.2×10^{-4} is greater than 0.01; (bottom) regions where the probability of ammonia mass fraction surpassing 2.2×10^{-4} is greater than 0.1.

Dr Yangyang LIU

CN14: Alternative marine fuel engine modelling

Prof Epaminondas MASTORAKOS (CAM)

Dr B HARIKRISHNAN (Research Fellow, CARES) has been actively involved in enhancing the capabilities of the in-house solver **dcmc-Converge** to address spray combustion problems. To test its efficacy, the solver was employed to perform a numerical investigation of the dual-fuel UCAM bluff-body stabilised swirl flame experiment (Figure 4.9). This experiment utilises n-heptane as a liquid fuel, which is injected in the presence of a methane/air premixed gaseous mixture. The mixture passes through a swirler before entering the combustion chamber via an annular passage. Such configurations are critical for understanding staged combustion processes and evaluating the impact of fuel-switching in gas turbine systems.

The flame behaviour was examined under two distinct equivalence ratios for the premixed mixture, specifically below and above the lower flammability limit (LFL), with values of $\phi_{premixed} = 0.16$ and $\phi_{premixed} = 0.56$, respectively. As shown in Figure 4.10, an increase in the methane/air equivalence ratio results in the flame resembling a premixed flame more closely than a spray flame [1]. Furthermore, the OH concentration field depicted in Figure 4.11 provides insight into the flame anchoring location. As the premixed equivalence ratio increases, the flame's anchoring point shifts from the inner recirculation zone (IRZ) above the bluff-body towards the outer recirculation zone (ORZ).

A review paper titled "Applications and modelling of dual-fuel combustion" has been submitted to the 21st International Conference on Flow Dynamics (ICFD2024) in Sendai, Japan to be presented during the plenary talk by **Prof Epaminondas MASTORAKOS (PI, CARES).**

References

[1] Sidey, Jennifer A.M., and Epaminondas Mastorakos. 'Stabilisation of Swirling Dual-Fuel Flames'. *Experimental Thermal and Fluid Science* 95 (July 2018): 65–72. https://doi.org/10.1016/j.expthermflusci.2018.02.007.

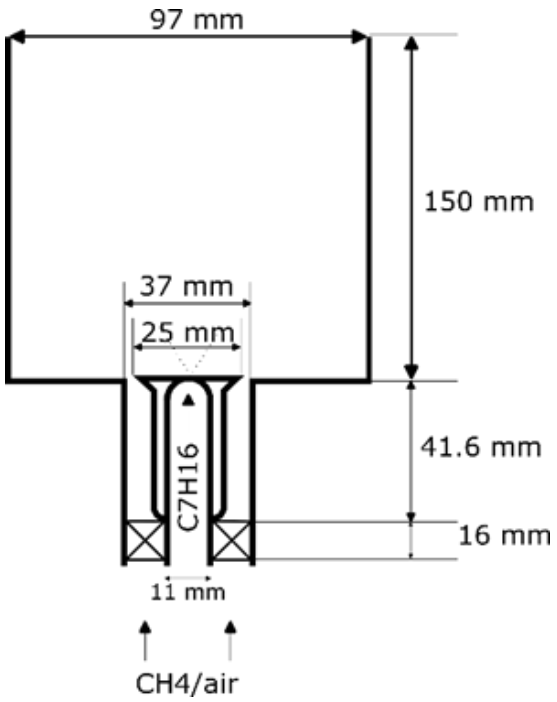


Figure 4.9: Schematic of the bluff-body stabilised swirl burner.

Dr B HARIKRISHNAN

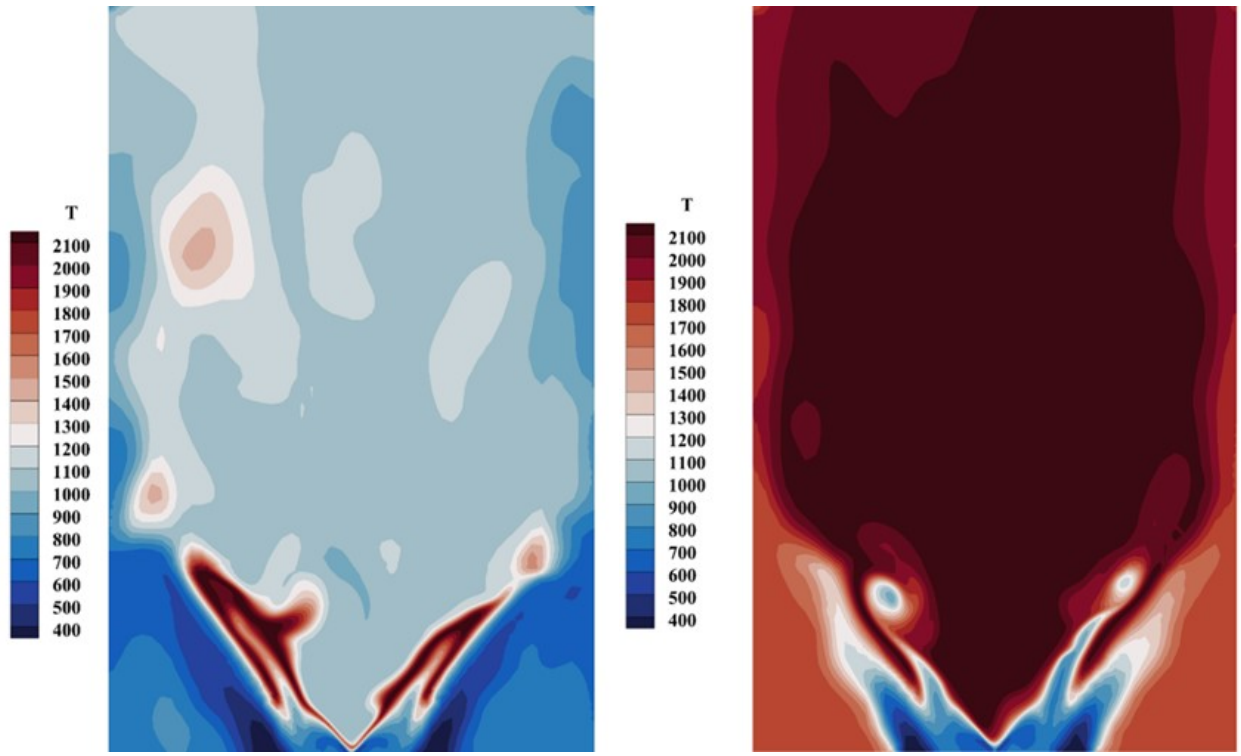


Figure 4.10: Temperature field.

Dr B HARIKRISHNAN

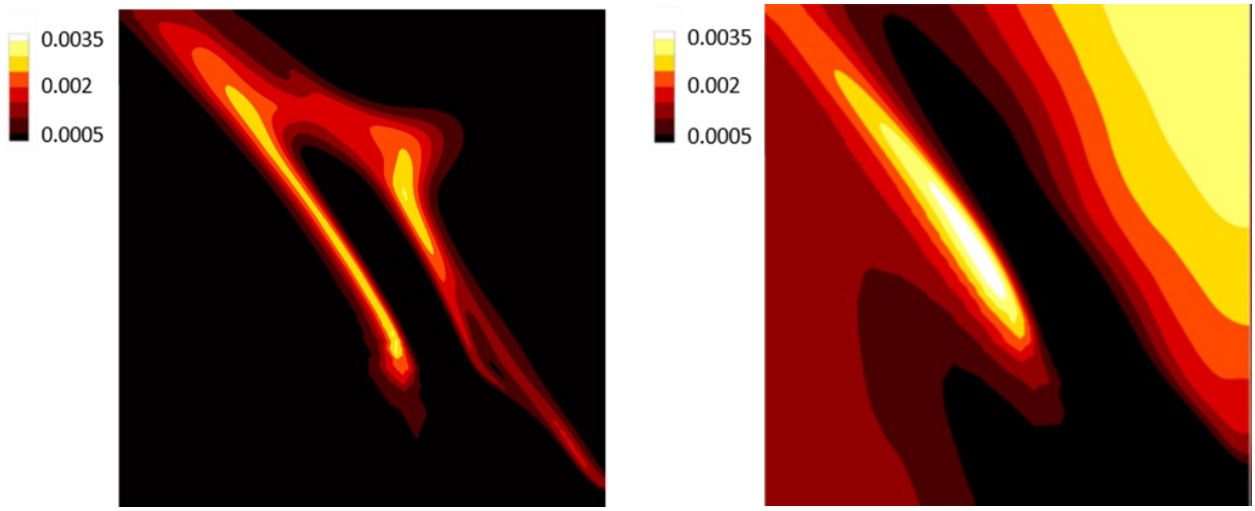


Figure 4.11: OH species concentration.

Dr B HARIKRISHNAN

CN16: Thermodynamics and process analysis of novel systems using the "cold energy" of liquid hydrogen to provide cooling needs and produce electricity

Prof Alessandro ROMAGNOLI (NTU)

Dr Mohamed Fadhel AYACHI (Senior Research Fellow, NTU) has been working on the utilisation of the high-grade cold energy content of both LNG and LH_2, exploring multiple utilisation opportunities such as in carbon capture and cryo-cogeneration. In this reporting period, the work provided a comparative techno-economic analysis of integrated process designs combining LNG cold utilisation with the most envisioned methods for CO_2 capture. These methods are:

- cryogenic carbon capture (with and without the use of N_2-selective membrane),
- chemical absorption carbon capture (using blended amine solvent MEA/MDEA),
- oxyfuel combustion (OFC) carbon capture (supported by a cryogenic O_2 production process),
- hybrid carbon capture involving steam methane reforming (SMR) and oxyfuel combustion (OFC).

The analysis refers to the LNG imports and distribution conditions in the city state of Singapore and sets the CO_2 capture at the limit of LNG cold utilisation. The steady-state thermodynamic models are developed at different levels of integration where the cold energy from LNG regasification can be utilised either in the CO_2 separation process, the CO_2 liquefaction process, or both processes. Liquefied carbon dioxide (LCO_2) at a low cryogenic temperature and a low pressure is the target output product in this analysis.

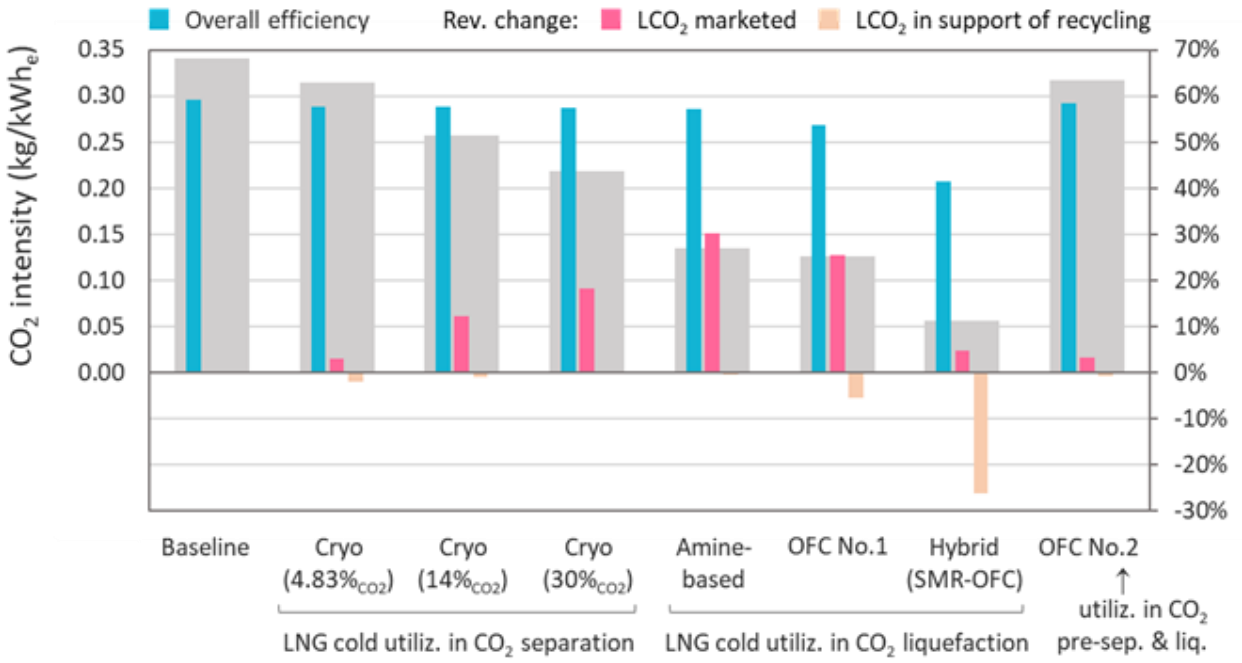


Figure 4.12: Comparative chart of the integrated process designs for LNG cold utilisation and CO_2 capture.

Dr Mohamed Fadhel AYACHI

The global LCO_2 market is not very large at present. It is focused on the food and beverage industry and accounted for approximately 16 Mtons in 2022. Considering this, the net revenue subject to an integrated process design is determined according to two case scenarios. The first case scenario assumes there is potential access to market where the derived LCO_2 product can be subject to commercialisation. The second case scenario assumes that, in the absence of market access, the LCO_2 product is made available at the maritime terminal as part of an initiative aimed at supporting the recycling and utilisation of carbon dioxide in catalytic conversion processes (e.g. thermocatalysis, electrocatalysis, etc.).

The net revenues from LNG-related power generation are then evaluated as part of the integrated systems in consideration, taking into account the associated operating costs for carbon capture, the environmental taxation policy, and the theoretical sale or non-sale of the LCO_2 product. The comparative techno-economic analysis indicates that an integrated cryogenic capture system and an integrated amine-based chemical absorption capture system would result in the least adverse impact on net revenue from power generation (> -0.02 US$/kg$_{LCO2}$) and in CO_2 abatement rates of up to 37.7% and 61.8%, respectively.

CARBON POLICY

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

Prof S VISWANATHAN (NTU)

Dr J. Lemuel MARTIN (Research Fellow, NTU) continues to work with **Prof S. VISWANATHAN (PI, NTU)** on business model innovations related to clean technology adoption, focusing on alternative solar business models. Numerical simulations on the multiple customer model have led to further refinement of previous results. We find that the separating condition wherein each third-party business model (leasing and PPA) is distinct depends not only on the heterogeneous characteristics of the customers (e.g., solar generation and electricity consumption) but also on the price ratio between the two models. The manuscript is now being updated to reflect these findings and their implications. **Dr Yan WANG (Research Fellow, NTU)** continues to work with Prof Viswanathan on the manuscript for the paper "Sustainability Reporting Quality and Carbon Emissions Reduction: the Role of Chief Sustainability Officer" and is finalising the last section for submission.

Prof Viswanathan, Dr Martin, and Dr Wang continue work on studying carbon tax implementations and their downstream impact on the price of goods and services. A study is being conducted on the potential impacts of carbon taxes in inducing clean technology adoption for maritime shipping. The study focuses on the maritime fuel transition and estimates the adoption cost of several decarbonisation pathways using the current literature. These estimated adoption costs provide a baseline for establishing maritime carbon taxes that may make the clean technology switch economically appealing. An initial analysis of the potential downstream impact of this carbon tax implementation on selected industries (steel, coal, crude oil) shows minimal impact on commodity prices. Further analysis is ongoing to investigate the implications of these results. The group is also conducting a similar analysis on the semiconductor industry, using data on electricity consumption and prices in Singapore, and is looking to expand this study to include the oil and gas industry.

DIGITAL NETWORKS

CN5: Introducing automated derivation and synthesis of high value molecules

Prof Markus KRAFT (CAM)
Prof Rong XU (NTU)

The project aims to develop the technology for automating the derivation of high value molecules based on existing knowledge through the representation and rational design of the molecules and the projection of their immediate chemical space. Reticular materials, such as Metal-Organic Frameworks (MOFs), Covalent Organic Frameworks (COFs), Metal-Organic Polyhedra (MOPs), Organic Cages, and zeolites, exhibit exceptional potential across various applications, including gas storage (notably for carbon dioxide and water vapour capture), separation processes, and catalysis. The project aims to emulate the rational design of these materials using The World Avatar (TWA), with the prospect of automating the synthesis of the proposed molecules using the next-generation laboratory.

During this reporting period, the team continued to advance the capabilities of the COF Construction Agent, generating over 20,000 COF geometries and thereby substantially expanding the existing dataset. In addition, utilising the COFmer Drawing Agent, machine-readable chemical string units were created to facilitate the prediction of key molecular features, such as hydrophobicity and hydrophilicity. These advancements facilitate the identification of common patterns and properties across different COF structures. The internal porosity and cavity characteristics of the COF structures have been calculated and represented within TWA.

Building on previous work related to the automated exploration of MOPs, the team updated the OntoMOPs ontology, incorporating over 370 new machine-predicted MOP geometries and restructuring the knowledge graph to reduce data redundancy and improve querying efficiency. Additionally, a natural language question-answering (QA) system was developed, employing few-shot in-context learning within its semantic parser, thereby allowing for more agile adaptation to new domains without the need for extensive retraining and improving the querying of MOP structures. The QA system also features retrieval-augmented generation (RAG) capabilities, which enables the generation of more contextually relevant and accurate responses, and is integrated with 3Dmol.js for the visualisation of complex chemical structures.

Finally, the team represented zeolitic formulations, their crystalline information, and molecular guests in a machine-actionable format using two newly developed ontologies, OntoCrystal and OntoZeolite, which were interconnected with OntoSpecies, the existing ontology for chemical species. This knowledge graph has been integrated with the QA system, demonstrating how structured information for reticular materials can be easily retrieved in natural language, eliminating the need for users to learn specialised query languages.

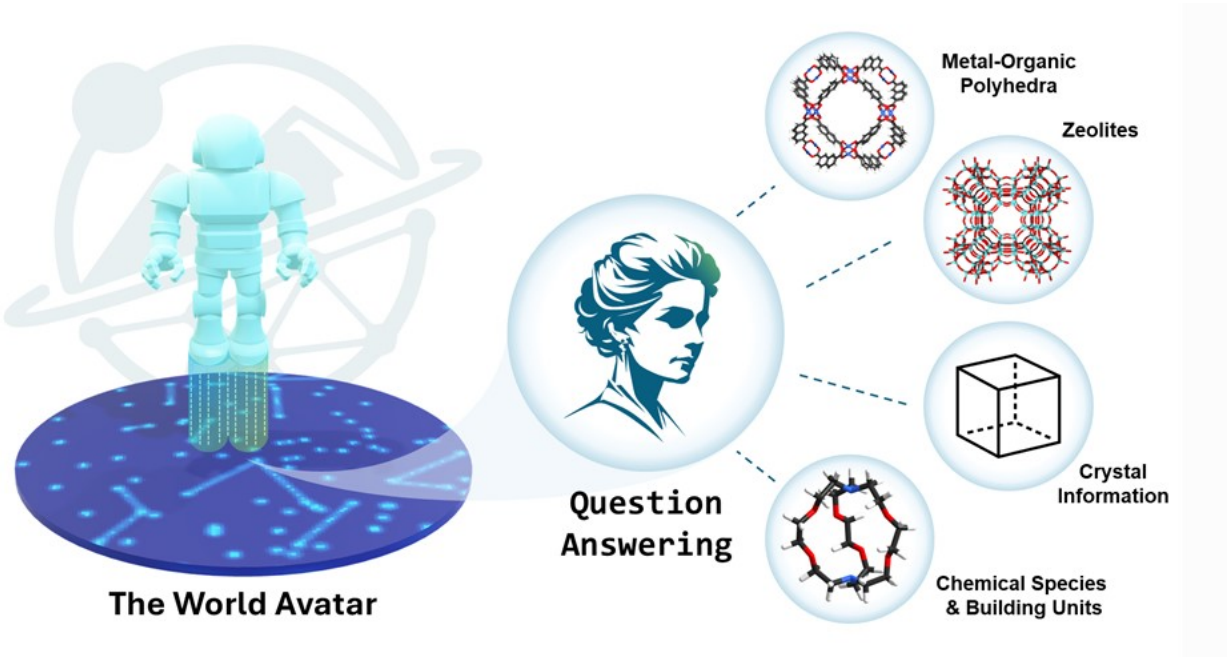


Figure 5.1: A knowledge graph interconnecting crystalline, zeolitic, chemical species, and building unit information with more abstract framework and assembly modelling information, and facilitating data curation through natural language processing.

CN23: Introducing next generation laboratory

Prof Markus KRAFT (CAM)

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

During this reporting period, the software infrastructure of the dynamic knowledge graph for The World Avatar (TWA) was consolidated and made available in the Python programming language. Leveraging remote control practices in laboratory automation, the knowledge graph is designed to operate over the internet, utilising deployment practices commonly employed by cloud-native applications, such as containerisation of microservice architecture. Figure 5.2 illustrates the distributed deployment philosophy for the self-driving laboratories. The triplestore and file server, which host the knowledge statements, are deployed at internet-accessible locations. Software agents are distributed across various host machines based on their capabilities, with agents responsible for hardware management located in the corresponding laboratories for security purposes. These agents facilitate data transmission between the hardware and the knowledge graph, and control the experimental equipment. Upon initialisation, agents register their instances within the knowledge graph using the OntoAgent ontology and autonomously execute their assigned tasks. Collectively, these agents form a distributed network that enables information exchange within the knowledge graph and with the equipment, effectively linking the digital twins with the physical world.

Furthermore, the team introduced a tool for the automated generation of topologies for novel reticular materials, such as Metal-Organic Polyhedra (MOPs), employing large language models (LLMs) to extract synthesis procedures compatible with the self-driving laboratories. To support this work, an ontology was developed to provide

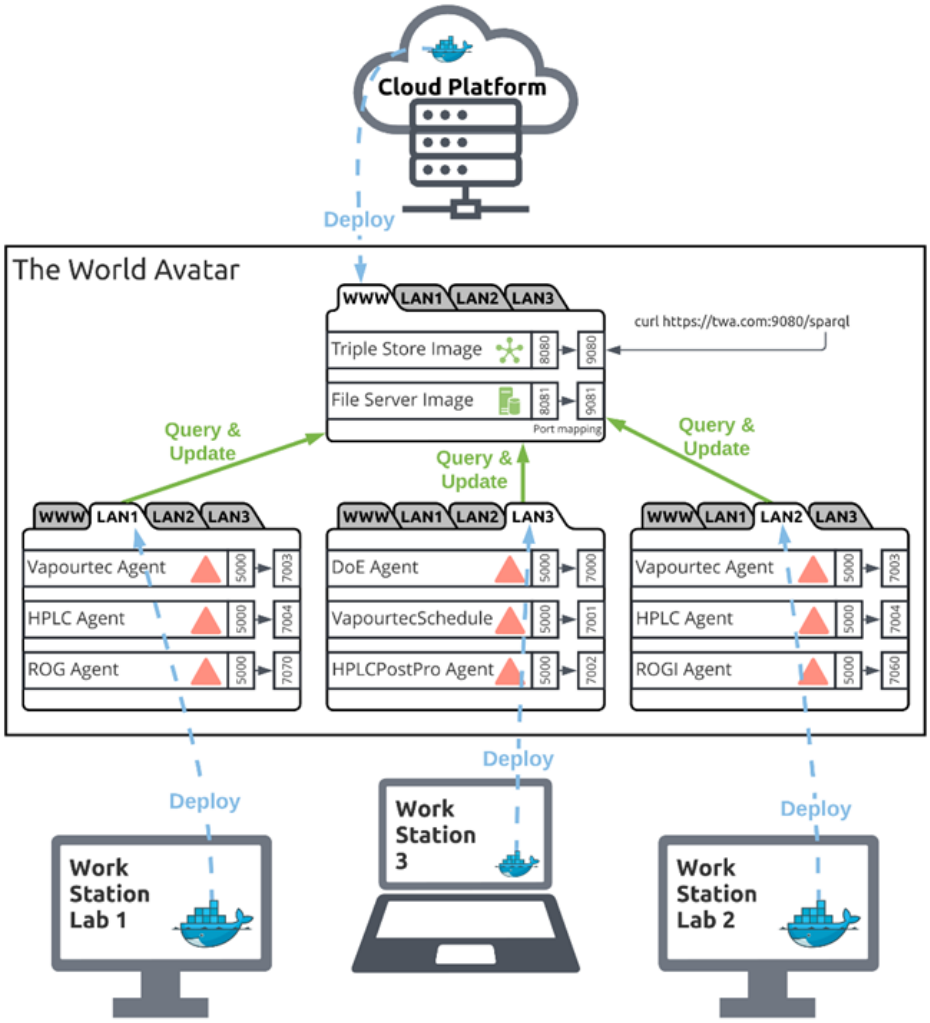


Figure 5.2: Schematic of the distributed deployment philosophy for self-driving laboratories.

a structured framework for representing both the topological features and synthesis procedures of MOPs. This ontology integrates key concepts, including chemical building units, assembly models, and reaction conditions, allowing for detailed annotation and querying of MOP data. By organising information on synthesis steps, reactants, and conditions within a hierarchical and interconnected schema, the ontology facilitates the extraction and reuse of synthesis procedures. Additionally, it supports the automation of synthesis by leveraging LLMs to parse and interpret synthesis protocols, ensuring that complex processes are accurately captured and can be reproduced or modified for new material designs.

CN24: Developing the Automated Lab of the Future

Prof Markus KRAFT (CAM)

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

During this reporting period, the team enhanced the features of both the Asset Management mobile application and the Augmented Reality (AR) application. These applications will enable users to access and manage laboratory data remotely, thereby improving the monitoring and control of laboratory operations and equipment. In the latest update to the Asset Management mobile application, the functionality for instantiating new assets into the knowledge graph has been fully implemented. This enhancement significantly streamlines the process of adding new assets, reducing the time required from the traditional 5 –10 minutes to approximately 3 minutes. The user workflow, depicted in Figure 5.3, follows a three-step process: It begins with the "Add Asset" option on the home screen (Figure 5.3(a)), where users are directed to a screen to enter or select relevant information about the new asset (Figure 5.3(b)). The subsequent screen allows users to verify and confirm the entered information (Figure 5.3(c)), after which the asset information is submitted for instantiation in the knowledge graph. A confirmation page is then displayed (Figure 5.3(d)), and a QR code is generated and queued for printing to be affixed to the newly added asset.

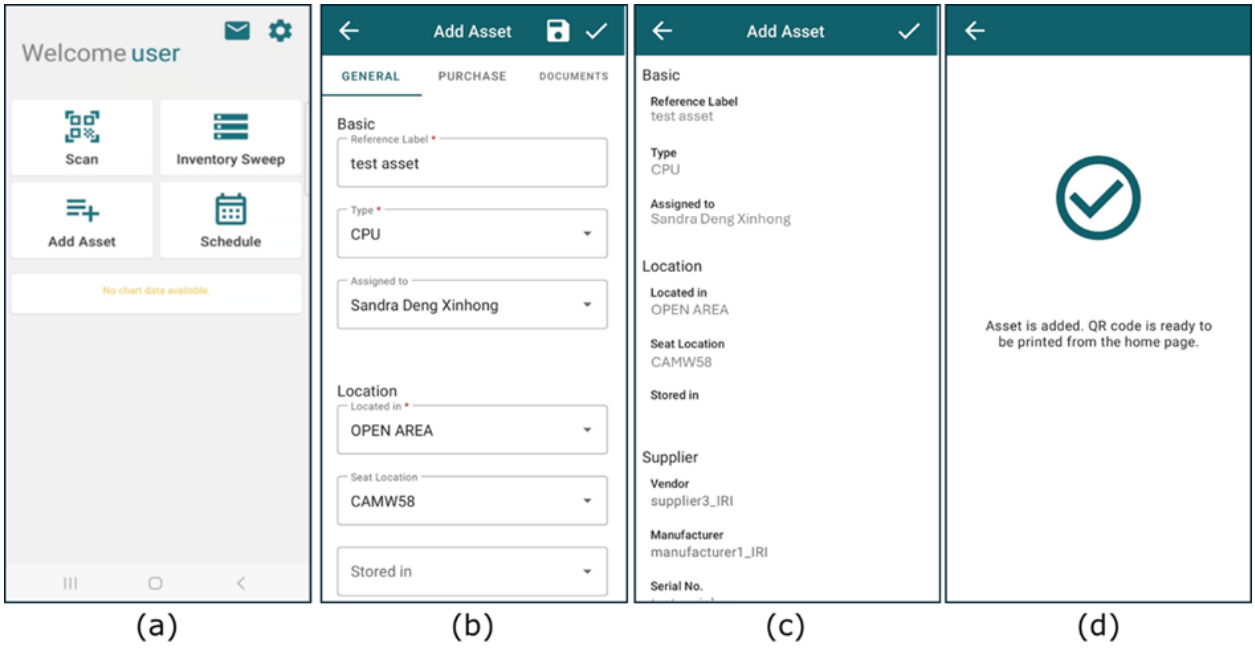


Figure 5.3: User experience workflow for the instantiation of new assets into the knowledge graph using the Asset Management mobile application.

Additionally, the team developed features within the AR application to enhance real-time laboratory management. The latest update includes the capability to monitor the contents of an explosive precursor cabinet. The user interface for this functionality is illustrated in Figure 5.4. Three-dimensional models of the explosive precursor cabinet were developed and integrated into the laboratory's floor plan. Figures 5.4(b), (c), and (d) demonstrate how users can access real-time information regarding the chemical bottles stored in the explosive precursor cabinet via the AR application, including detailed chemical information.

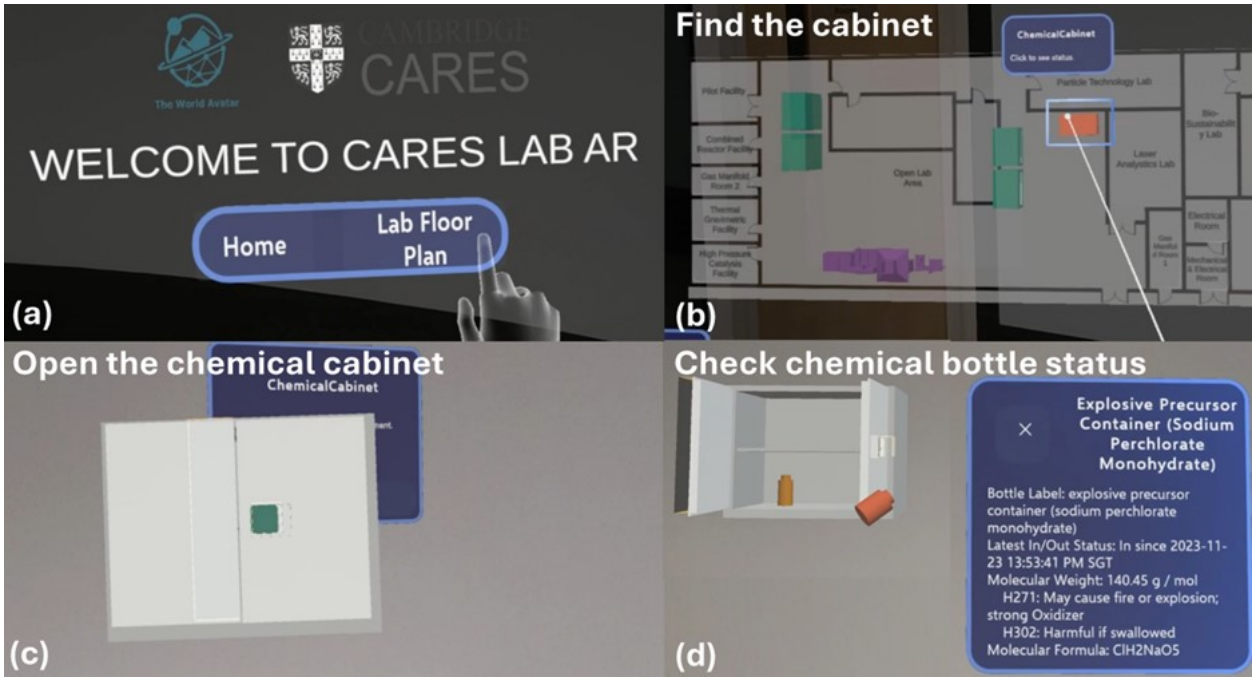


Figure 5.4: Augmented Reality application for the CARES laboratory, illustrating the monitoring of chemical bottles in the explosive precursor cabinet.

Scientific output

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

A simple and efficient approach to unsupervised instance matching and its application to linked data of power plants

Andreas Eibeck, Shaocong Zhang, Mei Qi Lim, and Markus Kraft, *Journal of Web Semantics*

DOI: 10.1016/j.websem.2024.100815

Abstract: Knowledge graphs store and link semantically annotated data about real-world entities from a variety of domains and on a large scale. The World Avatar is based on a dynamic decentralised knowledge graph and on semantic technologies to realise complex cross-domain scenarios. Accurate computational results for such scenarios require the availability of complete, high-quality data. This work focuses on instance matching — one of the subtasks of automatically populating the knowledge graph with data from a wide spectrum of external sources. Instance matching compares two data sets and seeks to identify instances (data, records) referring to the same real-world entity. We introduce AutoCal, a new instance matcher which does not require labelled data and runs out of the box for a wide range of domains without tuning method-specific parameters. AutoCal achieves results competitive to recently proposed unsupervised matchers from the field of Machine Learning. We also select an unsupervised state-of-the-art matcher from the field of Deep Learning for a thorough comparison. Our results show that neither AutoCal nor the state-of-the-art matcher is superior regarding matching quality while AutoCal has only moderate hardware requirements and runs 2.7 to 60 times faster. In summary, AutoCal is specifically well-suited to be used in an automated environment. We present its prototypical integration into the World Avatar and apply AutoCal to the domain of power plants which is relevant for practical environmental scenarios of the World Avatar.

Tailoring atomic chemistry to refine reaction pathway for the most enhancement by magnetization in water oxidation

Tianze Wu, Jingjie Ge, Qian Wu, and Zhichuan J. Xu, *Proceedings of the National Academy of Sciences*

DOI: 10.1073/pnas.2318652121

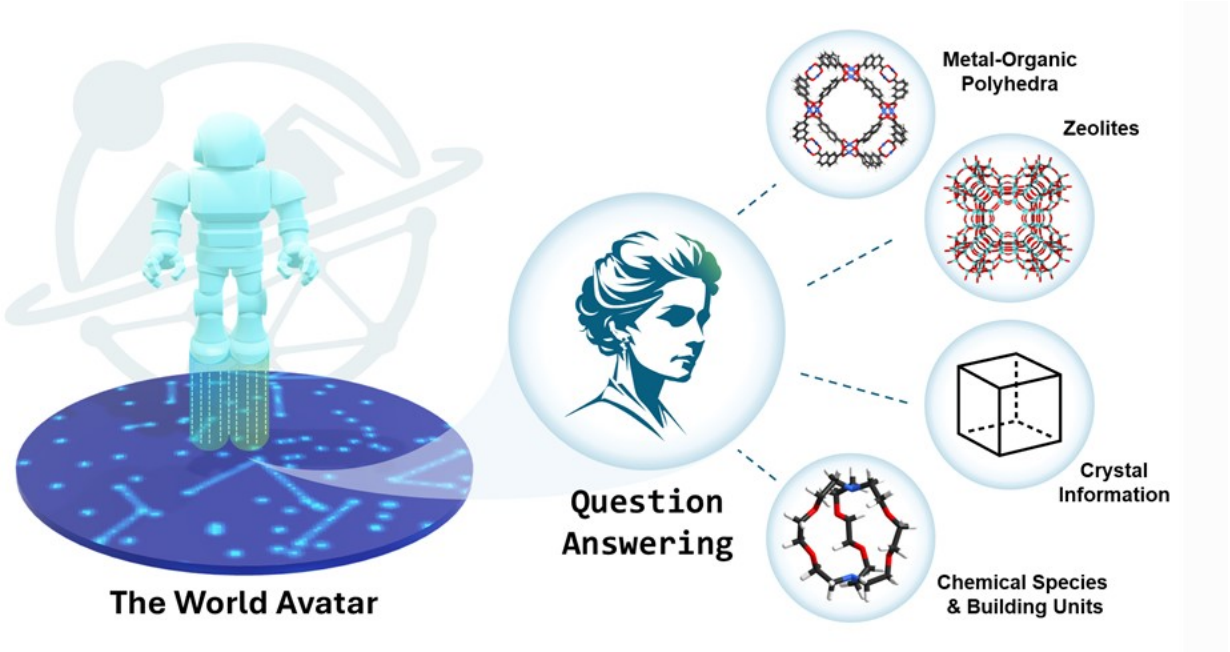
Abstract: Water oxidation on magnetic catalysts has generated significant interest due to the spin-polarization effect. Recent studies have revealed that the disappearance of magnetic domain wall upon magnetization is responsible for the observed oxygen evolution reaction (OER) enhancement. However, an atomic picture of the reaction pathway remains unclear, i.e., which reaction pathway benefits most from spin-polarization, the adsorbent evolution mechanism, the intermolecular mechanism (I2M), the lattice oxygen-mediated one, or more? Here, using three model catalysts with distinguished atomic chemistries of active sites, we are able to reveal the atomic-level mechanism. We found that spin-polarized OER mainly occurs at interconnected active sites, which favors direct coupling of neighboring ligand oxygens (I2M). Furthermore, our study reveals the crucial role of lattice oxygen participation in spin-polarized OER, significantly facilitating the coupling kinetics of neighboring oxygen radicals at active sites.

Knowledge graph representation of zeolitic crystalline materials

Aleksandar Kondinski, Pavlo Rutkevych, Laura Pascazio, Dan N. Tran, Feroz Farazi, Srishti Ganguly, and Markus Kraft, *Digital Discovery*

DOI: 10.1039/D4DD00166D

Abstract: Zeolites are complex and porous crystalline inorganic materials that serve as hosts for a variety of molecular, ionic and cluster species. Formal, machine-actionable representation of this chemistry presents a challenge as a variety of concepts need to be semantically interlinked. This work demonstrates the potential of knowledge engineering in overcoming this challenge. We develop ontologies OntoCrystal and OntoZeolite, enabling the representation and instantiation of crystalline zeolite information into a dynamic, interoperable knowledge graph called The World Avatar (TWA). In TWA, crystalline zeolite instances are semantically interconnected with chemical species that act as guests in these materials. Information can be obtained via custom or templated SPARQL queries administered through a user-friendly web interface. Unstructured exploration is facilitated through natural language processing using the Marie System, showcasing promise for the blended large language model – knowledge graph approach in providing accurate responses on zeolite chemistry in natural language.



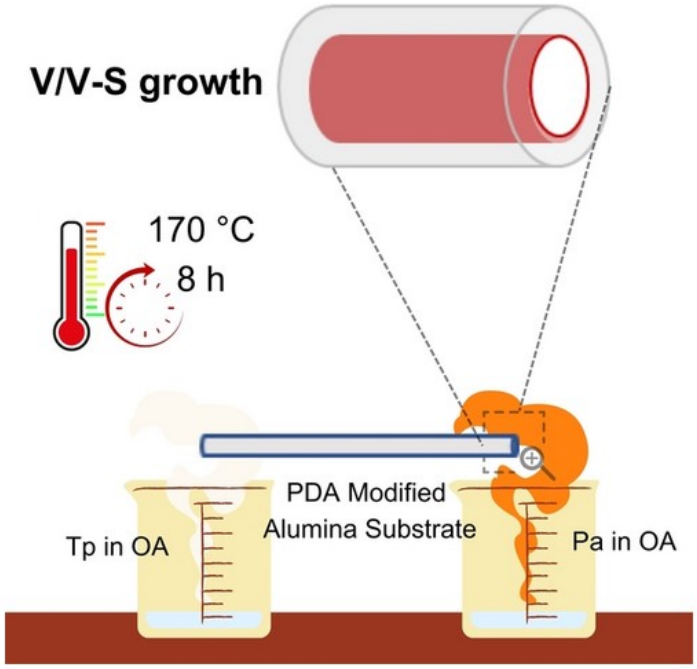
Vapor/Vapor-Solid Interfacial Growth of Covalent Organic Framework Membranes on Alumina Hollow Fiber for Advanced Molecular Separation

Wei Jian Samuel Siow, Jeng Yi Chong, Jia Hui Ong, Markus Kraft, Rong Wang, and Rong Xu,

Angewandte Chemie International Edition

DOI: 10.1002/anie.202406830

Abstract: Covalent organic frameworks (COFs), known for their chemical stability and porous crystalline structure, hold promises as advanced separation membranes. However, fabricating high-quality COF membranes, particularly on industrial-preferred hollow fiber substrates, remains challenging. This study introduces a novel vapor/vapor-solid (V/V–S) method for growing ultrathin crystalline TpPa-1 COF membranes on the inner lumen surface of alumina hollow fibers (TpPa-1/Alumina). Through vapor-phase monomer introduction onto polydopamine-modified alumina at 170 °C and 1 atm, efficient polymerization and crystallization occur at the confined V–S interface. This enables one-step growth within 8 h, producing 100 nm thick COF membranes with strong substrate adhesion. TpPa-1/Alumina exhibits exceptional stability and performance over 80 h in continuous cross-flow organic solvent nanofiltration (OSN), with methanol permeance of about 200 L m^{-2} h^{-1} bar^{-1} and dye rejection with molecular weight cutoff (MWCO) of approximately 700 Da. Moreover, the versatile V/V–S method synthesizes two additional COF membranes (TpPa2Cl/Alumina and TpHz/Alumina) with different pore sizes and chemical environments. Adjusting the COF membrane thickness between 100–500 nm is achievable easily by varying the growth cycle numbers. Notably, TpPa2Cl/Alumina demonstrates excellent OSN performance in separating the model active pharmaceutical ingredient glycyrrhizic acid (GA) from dimethyl sulfoxide (DMSO), highlighting the method's potential for large-scale industrial applications.

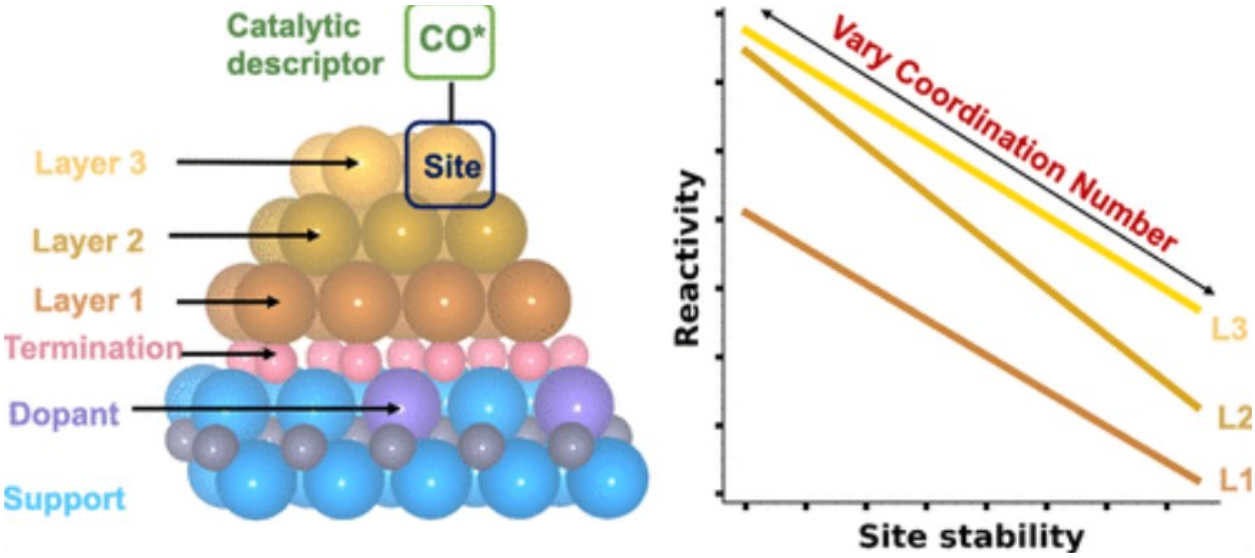


Generalized Principles for the Descriptor-Based Design of Supported Gold Catalysts

Lavie Rekhi, Quang Thang Trinh, Asmee M. Prabhu, and Tej S. Choksi, *ACS Catalysis*

DOI: 10.1021/acscatal.4c04049

Abstract: We postulate generalized principles for determining catalytic descriptors like the adsorption energy of CO*, across interfacial active sites of gold catalysts having varying coordination numbers and differing proximity to the support. These principles are derived using Density Functional Theory (DFT) calculations, linear scaling relationships, and an electronic structure analysis. Considered supports include two-dimensional (2D) and three-dimensional (3D) carbides and nitrides, doped MgO, and MoS_2. We show that the stability of gold atoms, across different coordination numbers, is linearly correlated to the adsorption energy of CO* through site-specific scaling relationships. As per definition, the slopes of these site-specific scaling relationships portray the extent of structure-sensitivity of CO* adsorption. This structure-sensitivity indicates the dependence of adsorption energies of CO* on the coordination number of the Au sites. The site-specific scaling relationships inform that interfacial perturbations are localized at the metal layer proximal to the interface. These perturbations are moreover strongest at low-coordinated gold sites. Interestingly, the interaction energies between adsorbates at higher coverages are insensitive to interfacial perturbations, further demonstrating the localized nature of metal–support interactions. Our interpretations of the slopes of site-specific scaling relationships indicate that the structure-sensitivity of interfacial gold sites is determined by the extent of interfacial charge transfer. The CO* adsorption energy is structure-insensitive on supports that induce a negative charge on interfacial gold atoms. This structure-sensitivity proportionally increases with the progressively increasing positive charge on interfacial gold atoms. Such charge transfer-dependent structure-sensitivity is rationalized using Lewis acid–base interactions. We demonstrate that tuning the adsorption energy of CO* by manipulating interfacial charge transfer can endow a Cu-like reactivity to interfacial Au sites for CO_2 electro-reduction. By melding the generalized principles derived in this study, we synthesize a scheme for determining site-specific catalytic descriptors at interfacial active sites of supported gold catalysts.

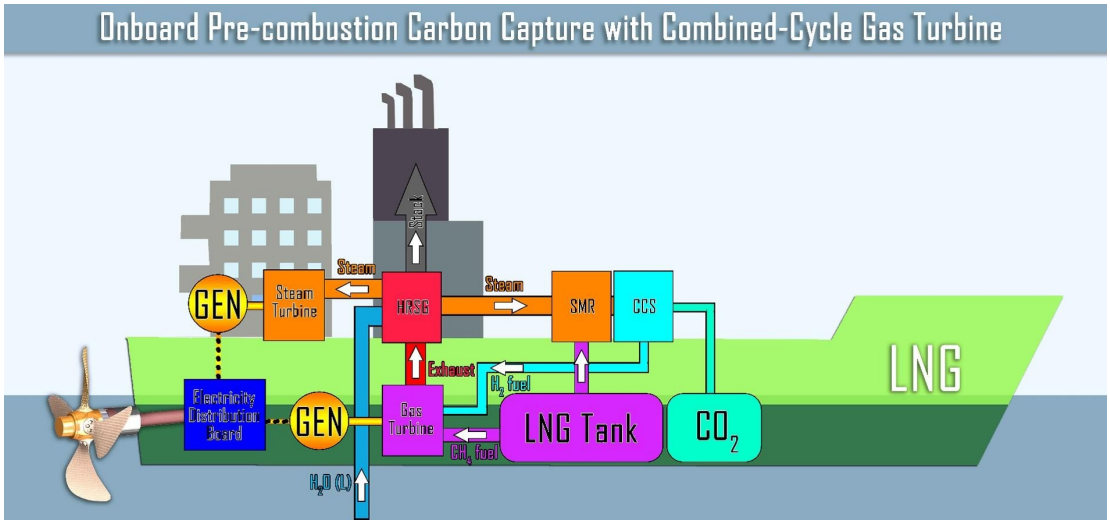


Onboard pre-combustion carbon capture with combined-cycle gas turbine power plant architectures for LNG-fuelled ship propulsion

Li Chin Law, Savvas Gkantonas, Agustin Mengoni, and Epaminondas Mastorakos, *Applied Thermal Engineering*

DOI: 10.1016/j.applthermaleng.2024.123294

Abstract: This paper investigates the concept of pre-combustion carbon capture (Pre-CCS) with a combined cycle gas turbine (CCGT) propulsion system to achieve energy efficient carbon capture onboard a Liquid Natural Gas fuelled vessel. A basic CCGT model with energy efficiency of 51.6 % when using LNG as fuel was integrated with a Pre-CCS system composed of a steam methane reformer, water–gas shift reactors, pressure swing adsorption (SMR-PSA), and liquid CO_2 storage. Various waste heat utilisation schemes integrated with the CCGT-reformer were modelled in Aspen HYSYS. The modelling of the waste heat recovery networks as energy streams integrating between various processes and unit of operations has facilitated a closed-loop simulation of various systems. It was concluded that a proper utilisation of the high-grade heat from the gas turbine (GT) exhaust and from the reformer is crucial to improve the overall energy efficiency and carbon capture rate, exemplified by a scheme where the heating needs for the SMR and the cooling needs from the water–gas-shift reactors are fully integrated. When optimised, the integrated system had an overall energy efficiency of 41.5 % and 43.2 % (i.e. an efficiency loss of 10.2–10.5 percentage points from the base CCGT system) accompanied with specific GHG emission reduction of 51.2 % and 52.3 % for operation of the GT at a turbine entry temperature of 1700 K and 1850 K, respectively. Intermediate levels of reforming, where the GT uses a mix of LNG and reformate gases, were also simulated, showing an almost linear evolution from the 100 % LNG feed to the GT to the 100 % reformate case. Such a strategy could be used for gradual evolution to meet the required CO_2 reduction timeline. It was determined that the 100 % reformate case provides the highest CO_2 capture rate. Estimates of other emissions from the GT assuming typical combustor residence times for the whole range of fuel blends were also carried out, showing that the overall greenhouse gas emission is dominated by CO_2, given that the GT emits negligible N_2O and unburnt methane. Some capital cost estimates were also made to determine the unit price of hydrogen fuel produced onboard, suggesting that the CAPEX was not prohibitive. These findings support the pre-combustion CCS – CCGT integrated system as a promising long-term decarbonisation and propulsion strategy to comply with emissions regulations, displaying good performance in terms of cost, energy consumption, and CO_2 reduction. The scalability and adaptability of the proposed system for existing and new-built ships across the decarbonisation timeline is also discussed.

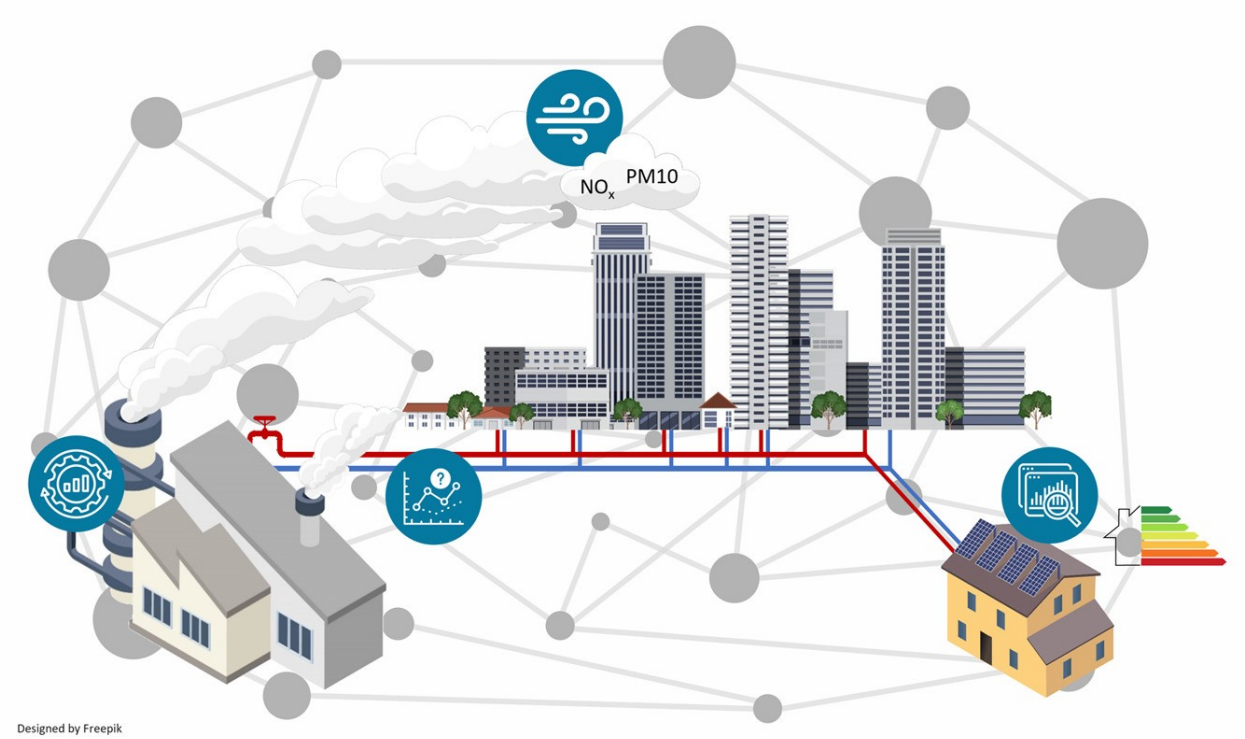


Dynamic control of district heating networks with integrated emission modelling: A dynamic knowledge graph approach

Markus Hofmeister, Kok Foong Lee, Yi-Kai Tsai, Magnus Müller, Karthik Nagarajan, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *Energy and AI*

DOI: 10.1016/j.egyai.2024.100376

Abstract: This paper presents a knowledge graph -based approach for the dynamic control of a district heating network with integrated emission dispersion modelling. We propose an interoperable and extensible implementation to forecast the anticipated heat demand of a municipal heating network, minimise associated total generation cost based on a previously devised methodology, and couple it with dispersion simulations for induced airborne pollutants to provide automatic insights into air quality implications of various heat sourcing strategies. We create cross-domain interoperability in the nexus of energy and air quality via newly developed ontologies and semantic software agents, which can be chained together via The World Avatar dynamic knowledge graph to resemble the behaviour of complex systems. Furthermore, we integrate the City Energy Analyst into this ecosystem to provide building-level insights into energy demand and renewable generation potential to foster strategic analyses and scenario planning. Underlying calculations use building and weather data from the knowledge graph in place of inherent assumptions in the official software release, facilitating a more data-driven approach. All use cases are implemented for a mid-size town in Germany as a proof-of-concept, and a unified visualisation interface is provided, allowing for the examination of 3D buildings alongside their corresponding energy demand and supply time series, as well as emission dispersion data. With this work, we outline the potential of Semantic Web technologies to connect digital twins for holistic energy modelling in smart cities, thereby addressing the increasing complexity of interconnected energy systems.

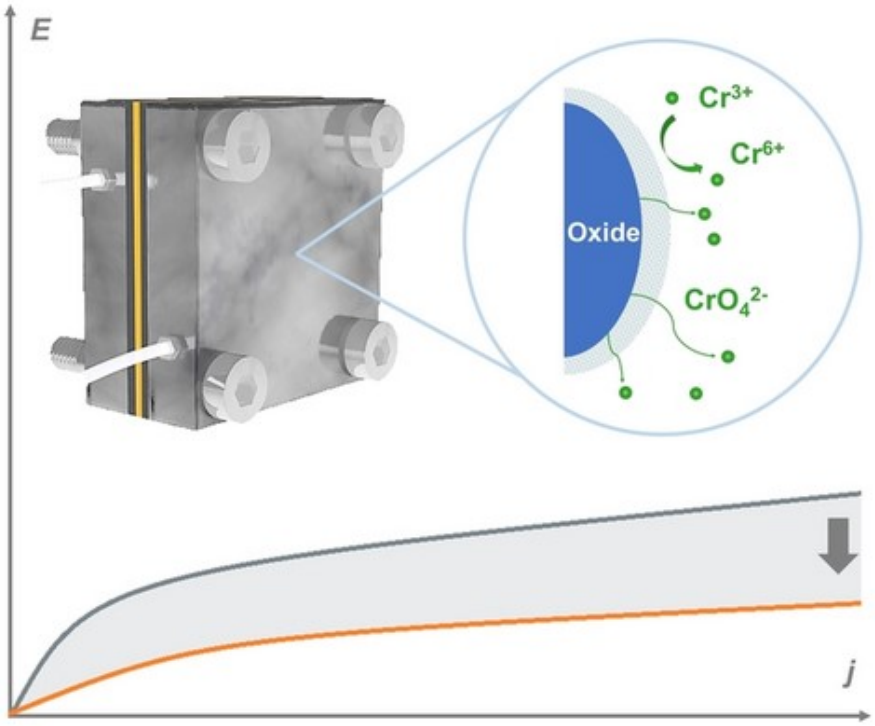


Elevated Water Oxidation by Cation Leaching Enabled Tunable Surface Reconstruction

Songzhu Luo, Chencheng Dai, Yike Ye, Qian Wu, Jiarui Wang, Xiaoning Li, Shibo Xi, and Zhichuan J. Xu, *Angewandte Chemie International Edition*

DOI: 10.1002/anie.202402184

Abstract: Water electrolysis is one promising and eco-friendly technique for energy storage, yet its overall efficiency is hindered by the sluggish kinetics of oxygen evolution reaction (OER). Therefore, developing strategies to boost OER catalyst performance is crucial. With the advances in characterization techniques, an extensive phenomenon of surface structure evolution into an active amorphous layer was uncovered. Surface reconstruction in a controlled fashion was then proposed as an emerging strategy to elevate water oxidation efficiency. In this work, Cr substitution induces the reconstruction of $NiFe_xCr_{2-x}O_4$ during cyclic voltammetry (CV) conditioning by Cr leaching, which leads to a superior OER performance. The best-performed $NiFe_{0.25}Cr_{1.75}O_4$ shows a ~1500 % current density promotion at overpotential η=300 mV, which outperforms many advanced NiFe-based OER catalysts. It is also found that their OER activities are mainly determined by Ni : Fe ratio rather than considering the contribution of Cr. Meanwhile, the turnover frequency (TOF) values based on redox peak and total mass were obtained and analysed, and their possible limitations in the case of $NiFe_xCr_{2-x}O_4$ are discussed. Additionally, the high activity and durability were further verified in a membrane electrode assembly (MEA) cell, highlighting its potential for practical large-scale and sustainable hydrogen gas generation.



Urban Vulnerability Assessment of Sea Level Rise in Singapore through the World Avatar

Shin Zert Phua, Kok Foong Lee, Yi-Kai Tsai, Srishti Ganguly, Jingya Yan, Sebastian Mosbach, Trina Ng, Aurel Moise, Benjamin P. Horton, and Markus Kraft, *Applied Sciences*

DOI: 10.3390/app14177815

Abstract: This paper explores the application of The World Avatar (TWA) dynamic knowledge graph to connect isolated data and assess the impact of rising sea levels in Singapore. Current sea level rise vulnerability assessment tools are often regional, narrow in scope (e.g., economic or cultural aspects only), and are inadequate in representing complex non-geospatial data consistently. We apply TWA to conduct a multi-perspective impact assessment of sea level rise in Singapore, evaluating vulnerable buildings, road networks, land plots, cultural sites, and populations. We introduce OntoSeaLevel, an ontology to describe sea level rise scenarios, and its impact on broader elements defined in other ontologies such as buildings (OntoBuiltEnv ontology), road networks (OpenStreetMap ontology), and land plots (Ontoplot and Ontozoning ontology). We deploy computational agents to synthesise data from government, industry, and other publicly accessible sources, enriching buildings with metadata such as property usage, estimated construction cost, number of floors, and gross floor area. An agent is applied to identify and instantiate the impacted sites using OntoSeaLevel. These sites include vulnerable buildings, land plots, cultural sites, and populations at risk. We showcase these sea level rise vulnerable elements in a unified visualisation, demonstrating TWA's potential as a planning tool against sea level rise through vulnerability assessment, resource allocation, and integrated spatial planning.

The digital lab manager: Automating research support

Simon D Rihm, Yong Ren Tan, Wilson Ang, Markus Hofmeister, Xinhong Deng, Michael Teguh Laksana, Hou Yee Quek, Jiaru Bai, Laura Pascazio, Sim Chun Siong, Jethro Akroyd, Sebastian Mosbach, and Markus Kraft, *SLAS Technology*

DOI: 10.1016/j.slast.2024.100135

Abstract: Laboratory management automation is essential for achieving interoperability in the domain of experimental research and accelerating scientific discovery. The integration of resources and the sharing of knowledge across organisations enable scientific discoveries to be accelerated by increasing the productivity of laboratories, optimising funding efficiency, and addressing emerging global challenges. This paper presents a novel framework for digitalising and automating the administration of research laboratories through The World Avatar, an all-encompassing dynamic knowledge graph. This Digital Laboratory Framework serves as a flexible tool, enabling users to efficiently leverage data from diverse systems and formats without being confined to a specific software or protocol. Establishing dedicated ontologies and agents and combining them with technologies such as QR codes, RFID tags, and mobile apps, enabled us to develop modular applications that tackle some key challenges related to lab management. Here, we showcase an automated tracking and intervention system for explosive chemicals as well as an easy-to-use mobile application for asset management and information retrieval. Implementing these, we have achieved semantic linking of BIM and BMS data with laboratory inventory and chemical knowledge. Our approach can capture the crucial data points and reduce inventory processing time. All data provenance is recorded following the FAIR principles, ensuring its accessibility and interoperability.

Dynamic knowledge graph applications for augmented built environments through "The World Avatar"

Hou Yee Quek, Markus Hofmeister, Simon D. Rihm, Jingya Yan, Jiawei Lai, George Brownbridge, Michael Hillman, Sebastian Mosbach, Wilson Ang, Yi-Kai Tsai, Dan N. Tran, Soon Kang, William Tan, and Markus Kraft, *Journal of Building Engineering*

DOI: 10.1016/j.jobe.2024.109507

Abstract: The proliferation of digital building models in recent years has led to a corresponding rise in specialised, non-interoperable models. These models impede sustainable developments by forming data silos that hinder cross-application data exchange and knowledge discovery processes. Although Semantic Web solutions hold promise in addressing these silos, current approaches primarily focus on developing novel ontologies, yielding similar outcomes. But it is unclear how these methodologies could support broader knowledge discovery processes and application requirements. This paper addresses these research challenges by introducing a dynamic knowledge graph as implemented within The World Avatar for interoperable building models. We demonstrate its value through two distinct applications in urban energy management and laboratory automation. The dynamic knowledge graph revolves around a comprehensive structured knowledge model constructed from ontologies and agents. Ontologies semantically annotate data and represent domain knowledge and their relationships with standardised definitions. When augmented with an agent architecture, the resulting knowledge model can align stakeholder perspectives and accommodate the dynamic and scalable nature of urban data. Moreover, the dynamic knowledge graph fosters innovative human-machine interactions through visualisation interfaces to augment knowledge discovery processes in the built environment for greater efficiencies and innovation. As the knowledge model expands, users gain access to a broader spectrum of private and public data sources and technologies, while reducing integration barriers. This is especially pertinent for smaller and less influential entities like municipal and local governments with limited resources, who can realise substantial benefits at reduced costs.

Heterogeneous Electrochemical Carbon Dioxide Reduction in Aqueous Medium Using a Novel N4-Macrocyclic Cobalt Complex

Libo Sun, Tan Su, Adrian Fisher, and Xin Wang, *Small Methods*

DOI: 10.1002/smtd.202400627

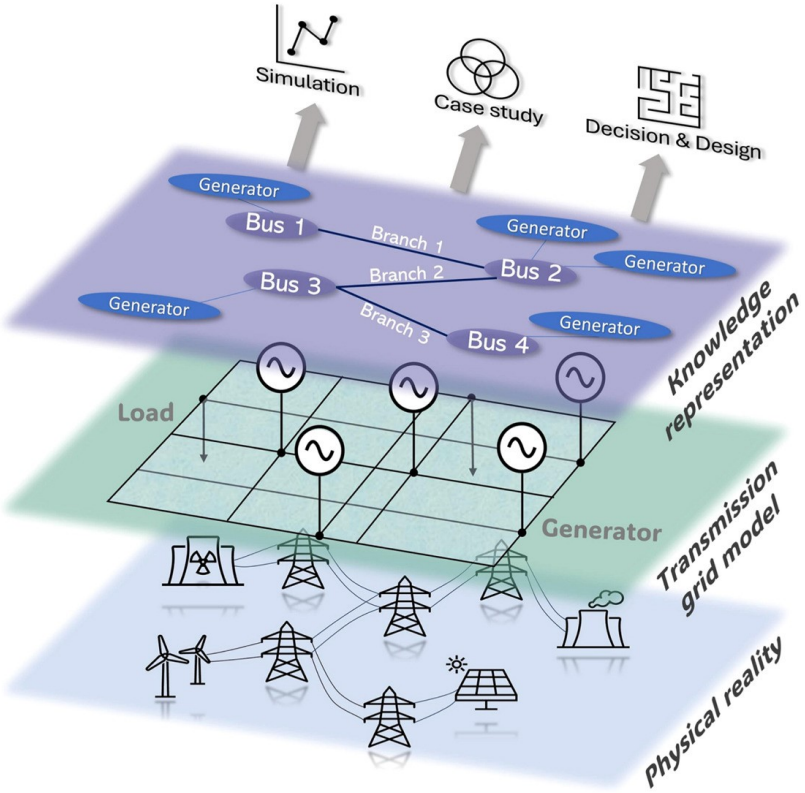
Abstract: Molecular catalysts represent an exceptional class of materials in the realm of electrochemical carbon dioxide reduction (CO_2RR), offering distinct advantages owing to their adaptable structure, which enables precise control of electronic configurations and outstanding performance in CO_2RR. This study introduces an innovative approach to heterogeneous electrochemical CO_2RR in an aqueous environment, utilizing a newly synthesized N4-macrocyclic cobalt complex generated through a dimerization coupling reaction. By incorporating the quaterpyridine moiety, this cobalt complex exhibits the capability to catalyze CO_2RR at low overpotentials and reaches near-unity CO production across a wide potential range, as verified by the online mass spectrometry and in situ attenuated total reflectance-Fourier transform infrared spectroscopy. Comprehensive computational models demonstrate the superiority of utilizing quarterpyridine moiety in mediating CO_2 conversion compared to the counterpart. This work not only propels the field of electrochemical CO_2RR but also underscores the promising potential of cobalt complexes featuring quaterpyridine moieties in advancing sustainable CO_2 conversion technologies within aqueous environments.

Dynamic knowledge graph approach for modelling the decarbonisation of power systems

Wanni Xie, Feroz Farazi, John Atherton, Jiaru Bai, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft,
Energy and AI

DOI: 10.1016/j.egyai.2024.100359

Abstract: This paper presents a dynamic knowledge graph approach that offers a reusable, interoperable, and extensible framework for modelling power systems. Domain ontologies have been developed to support a linked data representation of infrastructure data, socio-demographic data, areal attributes like demand, and models describing power systems. The knowledge graph links the data with a hierarchical representation of administrative regions, supporting geospatial queries to retrieve information about the population within the vicinity of a power plant, the number of power plants, total generation capacity, and demand within specific areas. Computational agents were developed to operate on the knowledge graph. The agents performed tasks including data uploading, updating, retrieval, processing, model construction and scenario analysis. A derived information framework was used to track the provenance of information calculated by agents involved in each scenario. The knowledge graph was populated with data describing the UK power system. Two alternative models of the transmission grid with different levels of structural resolution were instantiated, providing the foundation for the power system simulation and optimisation tasks performed by the agents. The application of the dynamic knowledge graph was demonstrated via a case study that investigates clean energy transition trajectories based on the deployment of Small Modular Reactors in the UK.



A nuclear future? Small Modular Reactors in a carbon tax-driven transition to clean energy

Wanni Xie, John Atherton, Jiaru Bai, Feroz Farazi, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *Applied Energy*

DOI: 10.1016/j.apenergy.2024.123128

Abstract: The study investigated the effect of a CO_2 tax to encourage the adoption of Small Modular Reactors (SMRs) as an alternative to fossil fuels for power generation in the UK. The trade-offs of different SMR placement policy options with respect to the competing objectives of minimising transmission losses and population risk were investigated to understand the impact on the optimal placement and usage of SMRs at different carbon tax levels. Different assumptions about renewable power availability were explored. The study identified the most cost-effective number of SMRs per site and optimised the power flow for cost efficiency. Regardless of renewable power availability, a carbon tax in the range of £45–60/t was found to incentivise the full adoption of SMRs with a levelised cost of electricity of £60/MWh versus £0–20/t at £40/MWh. The SMR placement influenced the performance and cost of the energy system, as well as whether a region acted as a net importer or exporter of energy. The most cost-effective solutions were achieved by balancing transmission loss and population risk.

Reducing particulate matter emissions and investigating soot characteristics in CI engines using alcohol-based additives: An experimental analysis

Qiren Zhu, Yichen Zong, Yong Ren Tan, Jie-Yao Lyu, Xinyi Zhou, Yifeng Wu, Jianfeng Pan, Haili Liu, Song He, Wang Chen, Wenbin Yu, Wenming Yang, and Markus Kraft, *International Journal of Hydrogen Energy*

DOI: 10.1016/j.ijhydene.2024.08.345

Abstract: Mitigating the impact of fossil fuels in diesel engines is crucial for addressing environmental issues, and alcohol-based fuel additives play a pivotal role. As key carriers of hydrogen, these additives have attracted considerable attention for their potential to reduce our dependence on fossil fuels. This study investigates the impact of blending diesel with various alcohols—n-butanol, n-octanol, and ethanol—at blending ratios of 20 and 50 vol% on combustion characteristics, emissions, and soot nanostructure in a compression ignition (CI) engine. Blending with n-butanol and ethanol notably retarded ignition delay and shortened combustion duration, whereas n-octanol's influence was minimal. Emission analyses highlighted that alcohol additions generally curtail nitrogen oxides (NO_x) emissions, with 20 vol% n-butanol or n-octanol effectively diminishing unburned hydrocarbon (HC) emissions. An in-depth analysis of particulate matter (PM) emissions revealed that incorporating 50 vol% n-butanol or 20 vol% ethanol can significantly reduce PM emissions, achieving a reduction of up to 68% under various engine conditions. The examination of soot characteristics via Raman spectroscopy analysis highlighted an increased oxidative reactivity in soot particles when using n-octanol and ethanol blends. Additionally, soot samples obtained from alcohol-diesel blends displayed a heightened presence of C=O groups, as identified through Fourier-transform infrared (FT-IR) spectroscopy analysis. This research offers profound insights into the intricate effects of alcohol-diesel blending on engine combustion and emissions.

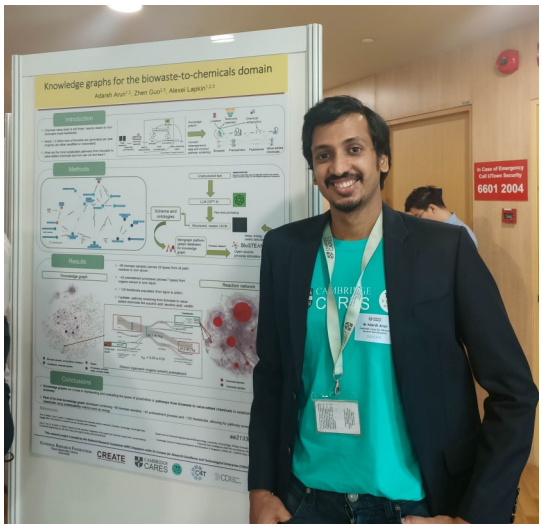
Other activities and achievements

Dr Li Chin LAW (Research Fellow, CARES), co-founder of the spin-off EMICAST, and The World Avatar project researchers had a shared decarbonisation booth at CREATE Symposium 2024 on Monday 22 July at NUS UTown. The booth was graced by Prof Tan Chorh Chuan, Permanent Secretary to the National Research Foundation Singapore and the event was an opportunity for CARES researchers to interact with the wider CREATE community.

Several posters were presented at CREATE Symposium 2024 in Singapore on 22 July 2024:

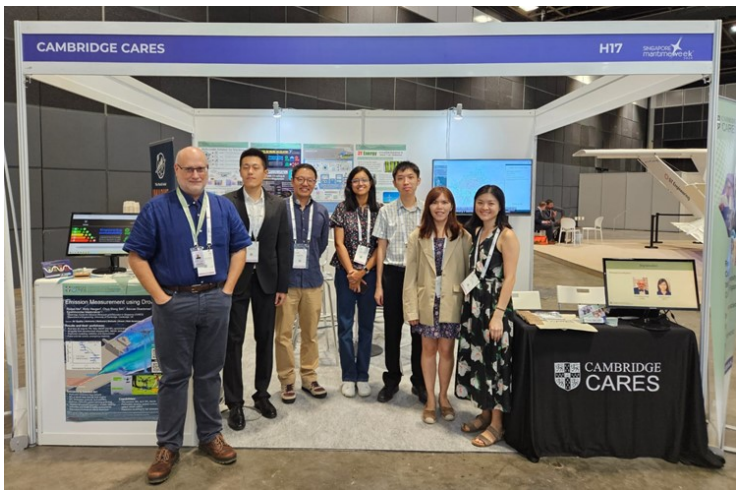
- **Dr Dogancan KARAN (Research Fellow, CARES)** presented "A Machine Learning-Enabled Process Optimisation of Ultra-Fast Flow Chemistry".
- **Dr Yichen ZONG (Research Fellow, NUS)** presented "Carbon neutral fuel additives for internal combustion engine".
- **Mr Adarsh ARUN (PhD student, CARES)** presented "Knowledge graphs for the bio-waste-to-chemicals domain"
- **Dr J. Lemuel MARTIN (Research Fellow, NTU)** presented "Logistics and Economics of Green Hydrogen-based Synthetic Fuel for Utilizing Captured CO_2".
- **Dr Kok Foong LEE (Software Developer, CARES)** presented "Simulating dispersion of pollutants from ships using The World Avatar"

The maritime decarbonisation group and digitalisation group had a shared booth at Singapore Maritime Week 2024 from 16-18 April at Suntec Convention & Exhibition Centre. The week-long event was attended by 17,000 participants from close to 80 countries, including high-level representation from governments, port authorities, and international organisations. Some of these organisations visited CARES and venture capital firms had engaging discussions with the CARES spin-offs 3Y Energy and EMICAST.



Photos from CREATE Symposium 2024:

Top left: Dr Li Chin Law (right) showing EMICAST to Prof Tan Chorh Chuan; Top right: Mr Adarsh Arun with his poster; Bottom left: The World Avatar researchers interacting with guests.



Photos from Singapore Maritime Week 2025:

Top: CARES researchers, Comms Manager (right) and PI Prof Epaminondas Mastorakos (left) at their booth; Bottom: Dr Li Chin Law and Dr Yichen Zong with the Chief Executive to the Maritime & Port Authority of Singapore, Mr Teo Eng Dih

Sustainable Reaction Engineering

The research team are actively collaborating with the company spun out of CARES in C4T Phase 2, Chemical Data Intelligence (CDI) Pte Ltd. It is intended that the CARES researchers, **Dr Zhen GUO (Senior Research Fellow, CARES)** and **Mr Adarsh ARUN (PhD student, CARES)** will become employees of CDI at the start of 2025.

Asst Prof Tej CHOKSI's (PI, NTU) group presented at these conferences:

- "Polarisation Effects at Metal/Support Interfaces Transcend Reactivity Constraints that are Ubiquitous in Oxygen Electrocatalysis" at the ACS Fall Meeting in Denver, USA from 18 - 22 August 2024.
- "How Structural Evolution during Strong Metal Support Phenomena Influences the Mechanism, Rate, and Selectivity of Formic Acid Decomposition" at the ACS Fall Meeting in Denver, USA from 18 - 22 August 2024.
- "The Influence of Strong Metal Support Interaction Phenomena on the Rates and Selectivity of Formic Acid Decomposition" at the 18th International Congress on Catalysis in Lyon, France from 14 - 19 July 2024.
- "Harnessing Ultrasound-derived Hydroxyl Radicals for the Selective Oxidation of Aldehyde Functions" at the 18th International Congress on Catalysis in Lyon, France from 14 - 19 July 2024.

Asst Prof Choksi was selected as a Young Talent Laureate at the 18th International Congress on Catalysis, one of the eminent meetings in the field of catalysis. 59 out of 392 applicants were given this label.

Maritime Decarbonisation

Dr Mutian MA (Research Fellow, CARES) delivered an oral presentation titled "The Use of Unmanned Aerial Vehicle in Detection of Pollution Dispersion and Transport Contributed by Mari-

time Emission in Singapore" at the joint 16th International Commission on Atmospheric Chemistry and Global Pollution/18th International Global Atmospheric Chemistry in Kuala Lumpur, Malaysia from 9-13 September 2024.

Dr Ma has also been in discussions with Fortescue engineers on the detection of ammonia engine emissions and safety measures for ammonia operation and storage.

Dr Li Chin LAW (Research Fellow, CARES) was invited by the Maritime & Port Authority of Singapore to join a GHG technical committee at an industry level.

Dr Yangyang LIU (Research Fellow, CARES) and **Prof Epaminondas MASTORAKOS (PI, CAM)** met with Seatrium to discuss the practical applications of their research in addressing ammonia leakage and bunkering scenarios on Friday 16 August 2024. During the meeting, Dr Liu presented their work titled "Computational Fluid Dynamics Simulation and Risk Assessment of Ammonia Leakage Scenarios During Ship-to-Ship Bunkering".

Digitalisation

Mr Simon RIHM (PhD student, CAM) presented "Advancing our mechanistic understanding of electrochemical CO_2 reduction with interconnected knowledge models" at the University of Cambridge's Chemical Engineering and Biotechnology (CEB) Conference from 2 - 3 July 2024.

Mr Dan TRAN (Software Developer, CARES) presented work from the paper "Natural Language Access Point to Digital Metal-Organic Polyhedra Chemistry in The World Avatar" (in preprint) at the Data-Centric Engineering (DCE) Workshop organised by The Alan Turing Institute at the IEEE Conference on Artificial Intelligence in Singapore on 25 June 2024.

Prof Markus Kraft gave presentations at the following events:

- "Question-answering system for combustion kinetics" at the 40th International Symposium on Combustion in Milan from 21 – 26 July 2024.
- "Building Resilient Cities with The World Avatar" at the International Conference on Resilient Systems in Singapore from 28 – 30 August 2024.
- "Decarbonization of energy systems using The World Avatar" at The Energy & Strategy Think Tank at WU Vienna University of Economics and Business, a partnership between VERBUND, Wien Energie and the Institute for Strategic Management (ISM).
- Presented The World Avatar and its applications in smart cities during the Urban Redevelopment Authority of Singapore's digital planning meeting on 17 May 2024.

CLIC

CENTRE FOR LIFELONG LEARNING AND INDIVIDUALISED COGNITION

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

Professor Annabel CHEN Shen-Hsing
Nanyang Technological University

Professor Zoe KOURTZI
University of Cambridge

OVERVIEW

The past six months have been an exciting period for CLIC. From a highly anticipated book launch to a series of symposiums, workshops and conferences. A highlight of this period was the production and launch of The Brainiverse Artbook, a creative spinoff from *The Brainiverse Experience* in 2023. Motivated by the overwhelming interest and enthusiasm from the special needs students who participated in the event, we compiled their artworks into a collection titled *Neurodiversity: No Brain is the Same*. The publication celebrates the connection between creativity and cognition, and the launch event provided a unique platform for students and teachers to share their stories with our guests and stakeholders. The event also featured a special commentary by Prof Trevor Robbins, who connected CLIC's research in neuroscience and creativity to the broader themes within the art book.

The researchers have been diligently analysing, drafting manuscripts, and submitting papers from Phase 1 of the project, resulting in several publications currently in progress across various workgroups. Alongside writing endeavours, the researchers have actively shared findings with the broader scientific community through paper and poster presentations at several conferences. A highlight of this was the series of Professional Development Workshop conducted at the Annual Meeting of the Academy of Management, where we showcased the application of advanced neuroscience methods such as functional magnetic resonance imaging and eye tracking.

The School team has made significant advances in the development of *Crossing Valley*, an innovative bridge construction game designed as a classroom tool to measure cognitive flexibility. The game has undergone multiple stages of testing and refinement, to ensure it effectively captures the cognitive process in an engaging manner. *Crossing Valley* is in its usability testing phase and the team is gathering valuable feedback from NTU students. The team is also working on a comprehensive data coding scheme for the game and are hoping to collaborate with machine learning experts from NTU to develop training models for data analysis, fostering an interdisciplinary approach to our research with cutting-edge technology.

The development of the Structure-Learning-Based Cognitive Flexibility Training Suite (SLiCX) is well underway, with ongoing and collaborative discussions across various workgroups. These efforts aim to enhance the cognitive battery and social measures in the adult sample and design an appropriate paradigm for adolescents. Despite encountering unforeseen delays, we will focus to move forward steadily. Pilot testing in both sample populations is planned for the upcoming months, and we are optimistic that the insights gained will greatly contribute to refining our task battery and training protocols.

Professor Annabel Chen Shen-Hsing
Director of CLIC, NTU

Professor Zoe Kourtzi
Director of CLIC, CAMBRIDGE

Update on Cognition Workgroup

Assessing Cognitive Flexibility, Other Executive Functions and Learning in Healthy Young Adults

Dr Ke TONG (Research Fellow, NTU) from the team has led the submission of the CLIC adult main manuscript (Broadening the Construct of Cognitive Flexibility) which highlighted the key findings of the CLIC Phase 1 adult study, revealing cognitive flexibility (CF) factors that are separable from other executive functions and general intelligence. Critically, cognitive flexibility factors were shown to predict outcomes like academic attainment, problem-solving, and creativity. Dr Tong and **Dr Xinchen FU (Research Fellow, NTU)** co-led a review paper on CF development, which was recently published in *Psychological Medicine*.

The first phase of the infant study has been successfully completed, and **Ms Natalie Philyra HOO (Research Assistant, NTU)** is currently assisting with data analysis and manuscript preparation. As Phase 2 of the study includes a new task battery, Ms Hoo has helped develop Standard Operating Procedures (SOPs) and adapted existing tasks to assess executive functions and creativity in infants which incorporates neurophysiological measures. She was also responsible for purchasing new interactive toys and study items, conducting dry-runs, and is actively recruiting new participants by liaising directly with interested mothers. Additionally, Ms Hoo set up data collection instruments on RedCAP for Phase 2 and collaborated with **Ms Winlynn CHOO (Research Associate, NTU)** to troubleshoot issues. The project is now live and ready for use.

Dr Fu is responsible in managing the testing sessions and analysis in the infant creativity testing and has been working on the data analysis and manuscript preparation of the infant exploratory studies. She contributed to the creativity foraging game data analysis in the adult dataset, where she explored connections between explore-exploit decision making and other cognitive abilities.

Mr Angshuk DUTTA (Research Assistant, NTU) joined the Cognition team in April 2024 and is responsible for data collection and data analysis in the current phase. His research also includes co-developing models with Dr Tong to extract features from participant drawings in the Torrance Tests of Creative Thinking Figural task and creating new metrics based on these features to understand figural creativity. Furthermore, under the guidance of **Prof Victoria LEONG (Co-Deputy Director and PI, NTU),** Mr Dutta is developing machine learning models to derive meaningful pose metrics from videos, specifically from tasks such as music play to determine original actions.

The following study has been pre-registered by the Cognition Workgroup on the Open Science Framework Registries.

Update on School Workgroup

Translation to Education: Assessing Cognitive Flexibility, Other Executive Functions and Learning in Healthy Adolescents

The School team, led by **Dr Nastassja LOPES FISCHER (Research Fellow, NTU),** is actively working on a series of papers focused on cognitive flexibility and creativity in adolescents. The abstract, Cognitive Flexibility and its Contribution to Originality in Divergent Thinking During Adolescence, has been accepted for presentation in November at the upcoming Psychonomics Conference 2024 in New York.

Dr Fischer, together with **Dr Nadhilla Velda MELIA (Research Fellow, NTU)** from the Social team, presented their results that explore the relationship between multilingualism and creativity from the adolescent and adult data at an Interdisciplinary Workshop on Multilingualism and Multiculturalism from 5-6 September titled 'The relationship between multilingualism and creativity from adolescence to adulthood'. The workshop was a fantastic opportunity to showcase CLIC's findings, and enabled researchers to engage and connect with experts from a range of fields (i.e., linguistics, sociology, machine learning, cultural psychology etc.) and meet potential collaborators for future research projects.

The School team has been actively involved in the development of the *Crossing Valley* game, an ecologically valid, classroom-relevant measure of cognitive flexibility within a problem-solving context. The game has undergone several stages of refinement and is currently in the usability testing phase with university students. A pilot study involving secondary school students in a focus group is scheduled for late September. The team is working on establishing the data coding scheme for *Crossing Valley*, including defining and coding for strategy switches. The team has also submitted a short paper on the development of *Crossing Valley* to be presented at the November Joint Conference on Serious Games 2024, in New York.

Two grant proposals stemming from this research have been submitted—a Science of Learning Grant (Ministry of Education) and an Education Research Funding Programme grant (Nanyang Technological University). These grants are a follow-up of the current research to extend the development of *Crossing Valley* and to identify and examine components of different teaching pedagogies (Knowledge Building, Contrasting Cases and Tinkering) on enhancing cognitive flexibility and learning outcomes in the classroom context. The team aims to address how lab-based cognitive flexibility observations translates to a classroom setting.

The School team has been collaborating closely with the Social team on papers that explore the relationship between multilingualism and creativity. The team found language entropy (balance between spoken languages) in adolescents to be negatively associated with originality scores in the Alternate Uses Test (AUT) – a measure of divergent thinking in creativity. This could be attributed to a limited vocabulary size for each spoken language in bilinguals compared to monolinguals, resulting in poorer performance in verbal creativity tasks compared to non-verbal tasks. Ongoing data analysis will help to understand what factors contribute to these observed associations and how different aspects of multilingualism could impact cognitive flexibility and creativity.

Work has advanced on validating the CLIP-Q (The Contextual Linguistic Profile Questionnaire) on the Singaporean adolescent population. The CLIP-Q is a holistic instrument designed to measure sociolinguistic diversity in different populations. The team assesses the instrument fit to Singapore's context, which helps understand how the language policies of Singapore and the shifting ecology towards English affects students' language use and choices.

Since 2022, the CLIC School Workgroup has been working with the Singapore Examination and Assessment Board (SEAB) on a project aimed at developing a measure for Critical, Analytical, and Inventive Thinking (CAIT) skills. The project entered its data collection phase in July, with an additional round to be conducted in October. This collaboration is crucial in understanding the translation of cognitive flexibility in the lab to real-life classroom settings in adolescents. In addition, the School Workgroup is planning to engage SEAB leaders to be involved in the co-creation of the *Crossing Valley* task.

Finally, the School team has been playing a supporting role in the development of SLiCX (Structure-Learning-Based Cognitive Flexibility Training Suite) by providing input on how to develop the SLiCX paradigm to be appropriate for adolescent testing.

The following study has been pre-registered by the School Workgroup on the Open Science Framework Registries.

Update on Social Workgroup

Cognitive Flexibility and Its Association with Linguistic Preferences, Decision-Making, Tolerance of Uncertainty and Perceived Social Support

The Social Workgroup have presented their results at various conferences and workshops in Singapore and the USA. The Social Workgroup has also been preparing manuscripts for publication on the social variables of multilingualism, social decision-making, the Big Five, and the relationships between these social variables as well as the relationship of these social variables with cognitive flexibility.

Prof Henriëtte HENDRIKS (Co-Deputy Director and PI, CAM) took up residency in Singapore from 1 April to 30 June 2024 to work closely with the Social and School Workgroups. The stay allowed her to attend the Artbook launch and workshop/mini conference by the Social Workgroup in which all postdocs and RAs had a chance to discuss their progress and findings regarding the various analyses undertaken. Prof Hendriks has contributed to the most recent paper on the Cognitive Flexibility construct, which was recently submitted after extensive revision. She has also been working regularly with Dr Melia on preparing papers related to multilingualism. Finally, she has also joined meetings with the School Workgroup on the social data and discussions regarding the relationship between multilingualism and creativity.

Prof Hendriks, with the support of **Prof Annabel CHEN (Co-Director and PI, NTU)** and **Assoc Prof Georgios CHRISTOPOULOS (PI, NTU)**, has also made connections with the Language and Communication Centre and the Modern Languages Centre of NTU to discuss cooperations which will allow the team to measure the advantages of learning a second language on executive functions and in particular cognitive flexibility with learners.

Dr Shengchuang FENG (Research Fellow, NTU) and **Dr Nadhilla Velda MELIA (NTU)** have both been working on several manuscripts related to the social factors and multilingualism. Dr Feng found a curvilinear relationship between cooperativeness and cognitive flexibility in his analysis of the WP 0.1 adult data and is conducting fur-

ther analysis to verify this. Meanwhile, he is collaborating with the Neuroimaging and School Workgroups in preparing the structure learning-based cognitive flexibility training suite (SLiCX) for WP 2.0. He is responsible for the development and implementation of social decision-making tasks in SLiCX and coding the structure learning task.

Ms Yoke Loo Emma SAM (PhD Student - IGP-CRADLE, NTU) is submitting her doctoral dissertation, which investigates cognitive functions – particularly cognitive flexibility and perceived competence – and how it is connected to practical outcomes (income and academic achievement) for working professionals and university students in Singapore.

Mr Akshay ABRAHAM (Research Associate, NTU) is helping with the preparation of social measures for the SLiCX study and assists in the coordination of Student Research Assistants as well as the organisation of academic talks by liaising with relevant parties. **Ms Hui Shan YAP (Research Assistant, NTU)** was involved in the Data Management Plan (DMP) discussion for studies in Phase 2. She was also involved in the analysis of the Big-5 personality data that was collected during multiple WP0 studies and has been helping with the manuscript draft. **Ms Yuan Ni CHAN (Research Assistant, NTU)** is in the process of assisting with the planning and the preparation of the social measures for the SLiCX study. **Ms Megan OH (Research Assistant, NTU)** is currently working on the manuscript from the data analysis of sleep quality, economic status, stress, and perceptions of economic status. Additionally, Ms Oh is assisting with the preparation for the SLiCX questionnaire for Phase 2.

The following study has been pre-registered by the Social Workgroup on the Open Science Framework Registries.

Update on Neuroimaging Workgroup

Neuroimaging: Structure Learning Training and Cognitive Flexibility

The Neuroimaging team has been collaborating with other workgroups to plan and design the Structure Learning (SL) training in Phase 2 as part of the Structure Learning-based Cognitive Flexibility Suite (SLiCX). To increase the difficulty in SL training, an additional dimension has been included to the task. The team has designed three pilot studies to investigate the saliency of the new dimension, progression criteria, and duration of training of the new SL task. Also, implicit and explicit instructions have been prepared to further examine the effectiveness of the training when participants are provided different styles of directions.

Pilot 1 has been developed and is pending deployment to the iABC platform which is undergoing migration. To mitigate delays in the study, a MATLAB alternative edited by **Mr Wei Ler KOO (Research Assistant, NTU)** and **Dr Shengchuang FENG (Research Fellow, NTU)** may be used for the pilot given the issues with the iABC platform. Scripts for Pilots 2 and 3 are also being developed ahead of the upcoming pilots. IRB documents have been submitted and approved for the pilot studies and recruitment has begun for pilot studies with both adult and adolescent participants. Once the migration of the iABC platform is complete, the team will begin the pilot study.

Dr Eleanor KOO (Research Fellow, NTU) is working with the other workgroups to confirm the tasks to be included on the cognitive task battery that would be implemented during Phase 2. The team are exploring different versions (e.g., in Python) of tasks currently hosted in Inquisit, to be deployed onto Azure for a centralised task battery. The cognitive task battery will be implemented during Pilot 3.

Dr Deepika SHUKLA (Research Fellow, NTU), supported by Dr Koo, Mr Koo, **Ms Winlynn CHOO (Research Associate, NTU)**, and **Ms Marisha UBRANI (Research Assistant, NTU)** has planned for a series of pilots to set up the Magnetic Resonance Imaging (MRI) data collection protocol to ensure high data quality and testing the SL task in the scanner. The scanner's remote controllers for the SL task were prepared and configured by Mr Koo and Ms Choo. An IRB amendment to include the first neuroimaging pilot has been prepared by Ms Ubrani and reviewed by Dr Shukla and Dr Koo. This includes the types of scans conducted, consent forms, questionnaires used, and strict screening measures to ensure participants' safety. An amendment has been submitted to the IRB, pending review and approval.

Dr Koo has carried out data quality check on the number of volumes in resting-state fMRI images and discovered multiple participants with missing volumes. This was conveyed to the Cognitive Neuroimaging Centre at NTU, and with the help of the radiographers, the team was able to recover the missing volumes. This brings the total number of participants to 103. Dr Koo has carried out pre-processing of the rsfMRI images and will be analysing them.

Dr Shukla has investigated the changes in magnetic resonance spectroscopy (MRS) derived metabolite levels among groups adopting different learning strategies on SL intervention. Relative change from pre-to-post training sessions have been analysed to assess the training induced metabolic modulation. Main effect of training ($p=0.006$) showed only training group to have significant reduction (mean diff: 0.842, $p=0.019$) of GABA+ level in R-DLPFC. Significant interaction effects ($p=0.049$) of group (training, control) and region of interest (ROI) (L- and R- DLPFC) were observed in the change (Δ: post-pre) of Glx level. Additionally, GABA+/Glx ratio was investigated to examine the relative balance of inhibitory to excitatory neurotransmission in cognitive flexibility. Significant main effect of ROI ($p=0.046$) on ΔGABA+/Glx ratio was observed, but post-hoc analysis did not show any significant group-wise differences ($p>0.5$). Decreased post-training R-DLPFC GABA+/Glx ratio and better SL performance post training suggest re-

duced effective inhibitory modulation through Inhibitory/Excitatory balance in R-DLPFC. No effect of group (p=0.674) and interaction with ROI (p=0.914) were observed. Association of inhibitory measures in R-& L-DLPFC with SL and CF scores suggests lateralised inhibition effect to govern the Learning performance in the training group. Dr Shukla and team also presented initial WP0.2 MRS data findings at various conferences in this reporting period.

The team has also extended the MRS data analysis to explore the hemispheric lateralisation effect on the training associated behavioural measures from the SL and CF tasks. Exploratory analysis on ΔGABA+/Glx ratio with SL strategy measure showed significant negative correlation of R-DLPFC ΔGABA+/Glx (r=-0.347; p=0.038) with SL training scores (Figure 6.1b). However, complementing positive relation (r=0.227, p=0.102) was observed with the L-DLPFC ΔGABA+/Glx in each training subgroup (Figure 6.1b). SL training induced metabolic modulation spreads over bilateral hemispheres, indicating improved cognitive flexibility in CST task. The work has been accepted for poster presentation for the upcoming Annual Meeting of the Society for Psychophysiological Research (SPR) in October.

Dr Shukla has been working on the MPM data processing and during initial data processing (Figure 6.1a) some data acquisition errors were

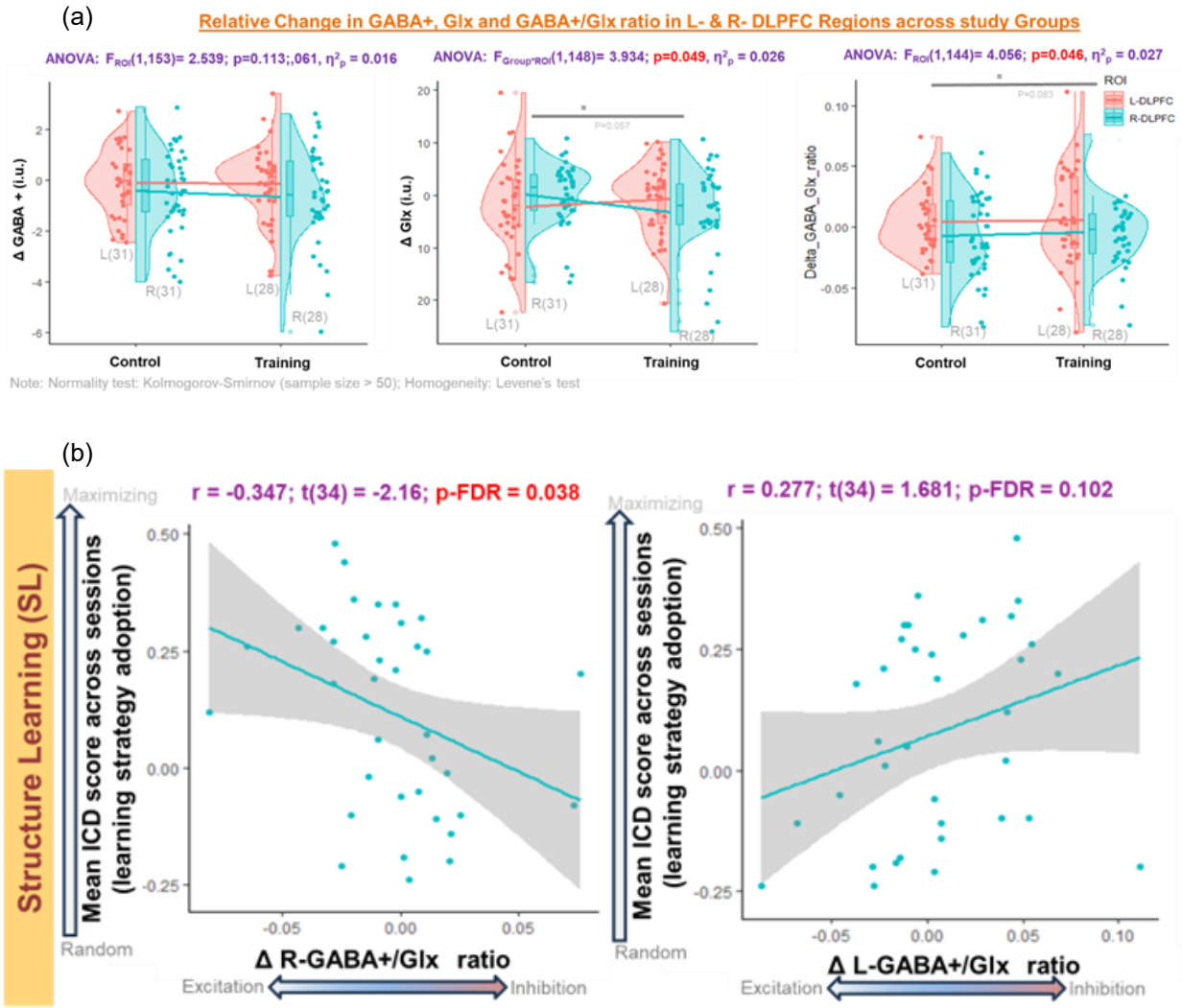


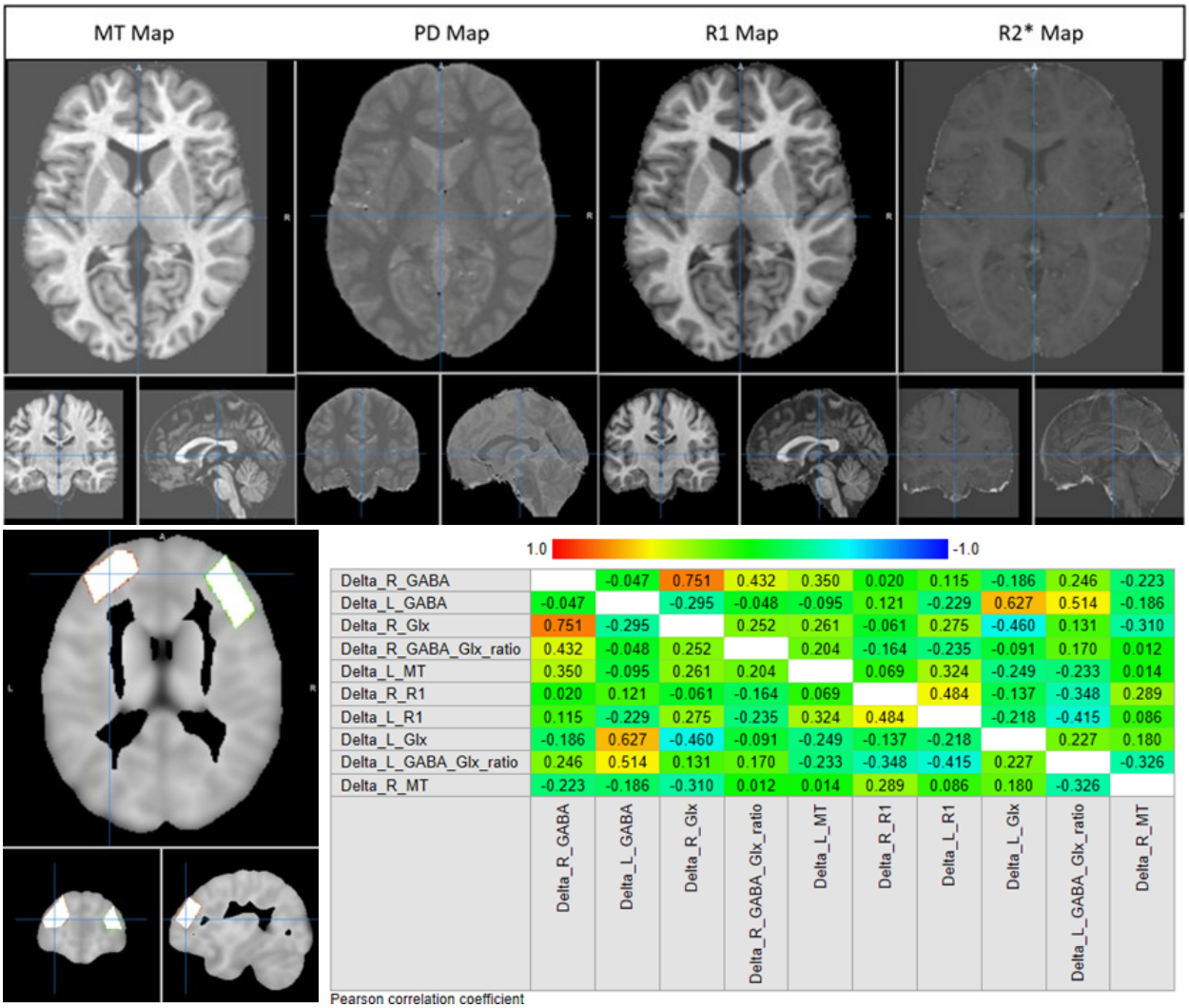
Figure 6.1: Neurochemical alterations in the (a) right (R)-DLPFC, and Left (L)- DLPFC ROI is between study groups and sessions. (b) Change in metabolic ratio in bilateral ROIs and their correlation with the Structure Learning.

identified on the body-coil maps which resulted in extended time in streamlining the data processing pipeline. Both MRS and MPM data processing on the WP0.2 dataset has now been completed along with a ROI analysis of the MPM data over MRS voxel masks (Figure 6.1b). Voxel based quantitation for whole brain analysis is in progress. The team aims to complete both MPM and MRS data analysis by the end of September.

Finally, the neuroimaging team's ethics application in Phase 1 was due for its annual review. A continuation review was prepared by Ms Ubrani and submitted to the Institutional Review Board (IRB) to allow the ongoing analysis of behavioural and neuroimaging data. The continuation review is still being processed by the IRB.

Currently, there are a few active trial projects built in REDCap: SLiCX for CLIC, BrainNorm and BrainNorm Project 5 for CRADLE, and Assessing Executive Function and Creativity in Infants for BabyLINC. This infrastructure development from CLIC has supported other Science of Learning projects within the university. In our tentative plan, the SLiCX project will act as a backup platform that centralises all behavioural data, and (semi-)automates result extraction from other platforms such as Qualtrics and Azure via API once the tasks are ready.

Led by CLIC's research engineer, **Dr Sheng Hung CHUNG (Research Engineer, NTU)** helps



	Delta_R_GABA	Delta_L_GABA	Delta_R_Glx	Delta_R_GABA_Glx_ratio	Delta_L_MT	Delta_R_R1	Delta_L_R1	Delta_L_Glx	Delta_L_GABA_Glx_ratio	Delta_R_MT
Delta_R_GABA		-0.047	0.751	0.432	0.350	0.020	0.115	-0.186	0.246	-0.223
Delta_L_GABA	-0.047		-0.295	-0.048	-0.095	0.121	-0.229	0.627	0.514	-0.186
Delta_R_Glx	0.751	-0.295		0.252	0.261	-0.061	0.275	-0.460	0.131	-0.310
Delta_R_GABA_Glx_ratio	0.432	-0.048	0.252		0.204	-0.164	-0.235	-0.091	0.170	0.012
Delta_L_MT	0.350	-0.095	0.261	0.204		0.069	0.324	-0.249	-0.233	0.014
Delta_R_R1	0.020	0.121	-0.061	-0.164	0.069		0.484	-0.137	-0.348	0.289
Delta_L_R1	0.115	-0.229	0.275	-0.235	0.324	0.484		-0.218	-0.415	0.086
Delta_L_Glx	-0.186	0.627	-0.460	-0.091	-0.249	-0.137	-0.218		0.227	0.180
Delta_L_GABA_Glx_ratio	0.246	0.514	0.131	0.170	-0.233	-0.348	-0.415	0.227		-0.326
Delta_R_MT	-0.223	-0.186	-0.310	0.012	0.014	0.289	0.086	0.180	-0.326	

Figure 6.2: MPM data analysis (top) An illustrative example of CLIC WP0.2 MPM data and processed Maps generated for further ROI-and group-based data analysis. Training induced change in MPM derived maps over the MRS ROIs. i.e. L and R-DLPFC. (Bottom-left) illustration of the two MRS ROIs on the MPM derived smoothed gray matter MTsat map. (Bottom-right) Correlation on the training induced changes (post-pre) of the MPM derived features with the MRS derived metabolite levels.

to oversee the CLIC server computing resources and CLIC data storage as illustrated in the Figure 6.3. In enhancing CLIC users' login security and accessing CLIC server computing resources, a server migration initiative with security enhancement has been carried out with the support of High-Performance Computing Centre (HPCC) at NTU to support the needs of secured, large-scale, compute and data intensive computation. All four CLIC servers have been migrated to HPCC in NTU and currently undergoing user setup and testing. In HPCC hosting, CLIC servers will be enhanced with OS Tuning and Optimization, Cluster and Nodes Integration, Application Support, License Server Hosting, and User Management.

As part of NTU Research Data Policy, a Data Management Plan (DMP) for CLIC is created in Research Information System (RISE) as part of NTU Research Data Policy. In managing the CLIC DMP, the Data Communication Team led by Dr Chung systematically records the steps in managing and using the research data. The DMP is reviewed and updated according to the changes in the research project to ensure accuracies and compliance.

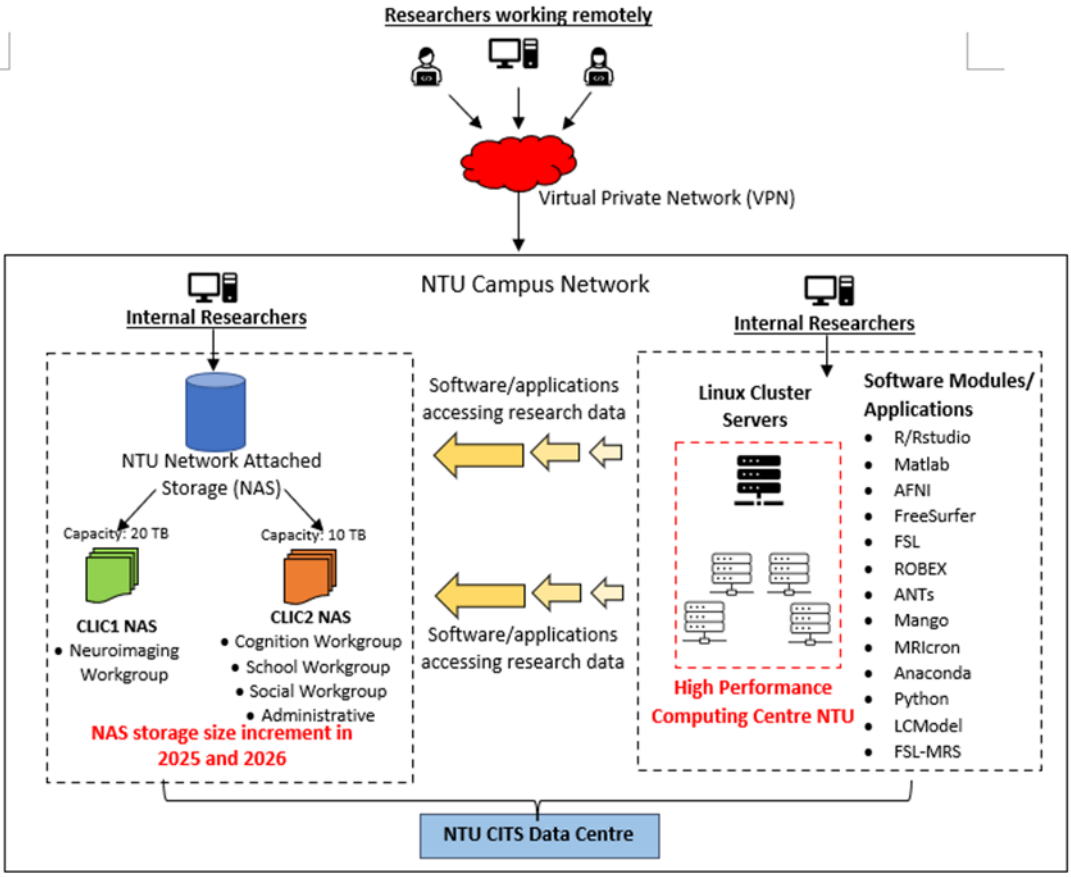


Figure 6.3: CLIC data storage and server computing infrastructure.

The following study has been pre-registered by the Neuroimaging Workgroup on the Open Science Framework Registries.

Scientific output

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

The Influence of Multilingual Experience on Executive Function and Structure Learning: Effects in Young Adults in the UK and Singapore

Chrysoula Vassiliu, Victoria Leong, and Henriëtte Hendriks, *Languages*

DOI: 10.3390/languages9040136

Abstract: Most studies regarding the relationship between multilingualism and cognitive control reduce linguistic diversity to a dichotomous comparison, viz., monolinguals vs. bilinguals, failing to capture the multifactorial nature of multilingualism. Language research is largely restricted to the Global North, albeit most of the world's population resides in the Global South, limiting the interpretability of the existing literature. Cognitive performance is assessed using very few tasks, yielding unreliable measurements. In this study, we identify the manner in which multilingual experiences influence cognitive performance in diverse sociolinguistic contexts. Young adults from the UK (n = 51, mean age = 24.0, SD = 3.18) and Singapore (n = 36, mean age = 21.3, SD = 2.15) were tested using an extensive battery of cognitive tasks, including cognitive flexibility (CF), working memory (WM), inhibition, and structure learning (SL). Information on language proficiency, use, age of acquisition, and frequency of switching was collected. The effects of various linguistic factors on the cognitive performance of each group were assessed using multiple linear regression models. The UK and Singapore samples exhibited significantly different linguistic profiles, which in turn dissimilarly influenced their cognitive performance. Our study underscores the necessity for more research in the Global South, challenging the prevailing Northern-centric focus on the multilingualism–cognition relationship.

Other activities and achievements

In August 2023, the CLIC team organised the highly successful *Brainiverse Experience: Jetting to Better Brain Health & Learning*. The team saw an overwhelming interest in the artwork submitted for the art competition themed "Neurodiversity: No Brain is the Same", which saw participation from students from special needs schools. This led to the Brainiverse Artbook which features selected submissions from the competition. The art book was officially launched on 21 May 2024 and guests had the opportunity to engage in hands-on activities used by neuroscientists to measure creativity. The event was organised by **Ms Marisha UBRANI (Research Assistant, NTU), Ms Phillis FU (Research Associate, NTU), Ms Restria FAUZIANA (Research Associate, NTU**) and **Dr Nadhilla Velda MELIA (Research Fellow, NTU)** from the various workgroups, and overseen by **Prof Henriëtte HENDRIKS (Co-Deputy Director and PI, CAM**). The event saw contributions and participation from all researchers at CLIC including a commentary on the relationship between creativity and cognition from **Prof Trevor ROBBINS (Senior Scientific Advisor, CAM).** Guests of Honours were also given a tour of the Lifespan Research Centre which hosts the BabyLINC laboratory, led by **Ms Natalie Philyra HOO (Research Assistant, NTU)**, sharing insights into ongoing studies and how EEG technology is used to study brain activity in infants, highlighting the methods and tools used in the research on cognitive development.

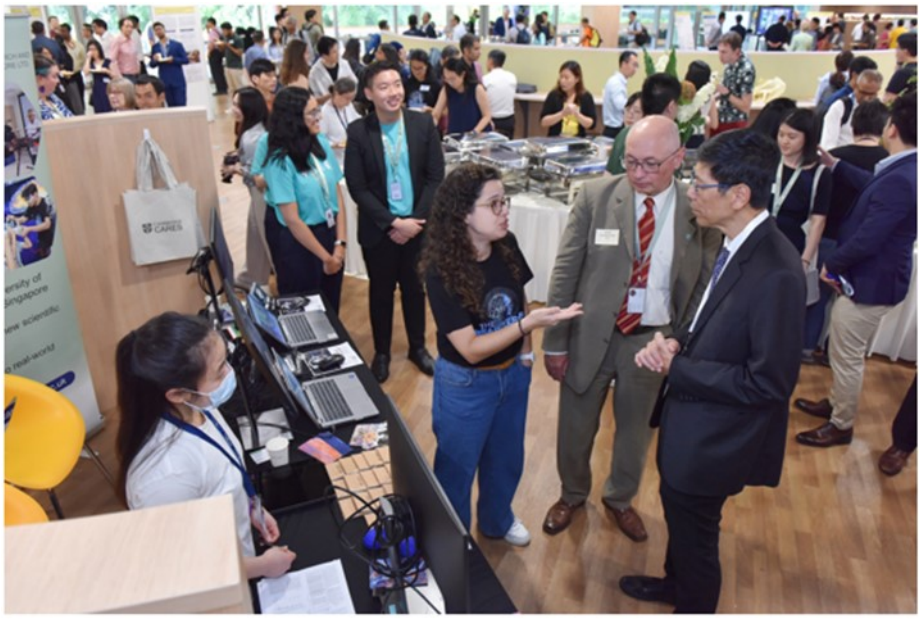
Guests of Honours Mrs Rosa Daniel (second from left) and Prof Shirley Ho (right) admiring the artwork on display during the artbook launch.

Prof Shirley Ho and Mrs Rosa Daniel (second and third from the left respectively) and Dr David Quach from the National Research Foundation (second from the right) listening to Ms Hoo explain the process of EEG capping on infants at the BabyLINC lab.

The CLIC team were also involved in CREATE Symposium on 22 July 2024, where they presented posters from the Neuroimaging, Social and Cognition team as well as a booth from the School team. The event was hosted by the National Research Foundation (NRF) and allowed for CLIC's research to be showcased to the various research partners in the CREATE programme.

Several posters were presented at the event:

- Dr Melia presented "Multilingualism and its Relation to Perceived Social Support and Cooperativeness".
- **Dr Deepika SHUKLA (Research Fellow, NTU)** presented "Neurochemical Alterations in Bilateral DLPFC in Response to Structural Learning Training in Healthy Adults".
- **Dr Ke TONG (Research Fellow, NTU)** presented "Broadening the Construct of Cognitive Flexibility and its Relevance to Academic Achievement and Creativity".



Dr Nastassja Lopes Fischer from the School Workgroup sharing the team's and CLIC's work to CARES Director Prof Markus Kraft (left) and NRF Permanent Secretary, Prof Tan Chorh Chuan.

Dr Shukla presented initial WP0.2 MRS data findings at various conferences:

- "Structure Learning Associated Bilateral DLPFC Excitatory/Inhibitory (Glx / GABA+) modulation in Healthy Adults" at the BrainConnects Joint Hybrid Neuroimaging Conference in Putrajaya, Malaysia from 7 - 8 June 2024.
- "Neurochemical Alterations in Bilateral DLPFC after Structure Learning Training in Healthy Adults" at the Annual Meeting Organization for Human Brain Mapping (OHBM) in South Korea from 23 - 27 June 2024.

Ms Yoke Loo, Emma SAM (PhD Student - IGP-CRADLE, NTU) presented her paper "Delving into the Underlying Dimensions of the Career Construction Model of Adaptation Among Singaporean Workers: A Psychometric Analysis" at the 6th Asian Management Research Consortium (AMRC) in Singapore from 26 - 27 April 2024.

Assoc Prof Georgios CHRISTOPOULOS (PI, NTU) organised three Professional Development Workshops at the 84th Annual Meeting of the Academy of Management (AOM 2024), a major academic event for management researchers, in Chicago USA from 9 - 13 August 2024. These were "Brain Imaging for Organizational Research: Hands-on Training for fMRI Studies", "Analysis of Heart Rate Responses for Manage-

ment Research", and "Eye-Tracking methods for Management Research"

The workshops focused on the use of neuroscience methods, including functional magnetic resonance imaging (conducted with **Dr Shengchuang FENG (Research Fellow, NTU)**), eye-tracking, and heart rate variability/ wearables. Assoc Prof Christopoulos also hosted Mr Jan RICHNER (PhD student, ETH Zurich) in August, who presented his work in cognitive flexibility and decision making in military leaders.

Dr Kastoori KALAIVANAN (Research Fellow, NTU) delivered a poster presentation "Communication Accommodation Theory and Dynamic Language Use in Multilingual Settings" at the Interdisciplinary Workshop on Multilingualism and Multiculturalism in Singapore from 5 - 6 September 2024. **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)** delivered an oral presentation "The relationship between multilingualism and creativity from adolescence to adulthood" at the same event.

The School Workgroup has been working closely with Singapore Examination and Assessment Board (SEAB) on the Critical, Analytical, and Inventive Thinking (CAIT) project. The team has also partnered with several local schools to involve them in CLIC's research and conducted outreach workshops for their educators.

The School Workgroup aims to collaborate with machine learning experts at NTU to train models to enhance the data analysis from *Crossing Valley*. The team has identified potential collaborators and will be inviting them to join the team effort.

The School Workgroup's findings on cognitive flexibility in adolescence has garnered keen interest from educators and the team have displayed their findings at the Science of Learning Education Centre noticeboard at the National Institute of Education (NIE) since June 2024. The School Workgroup have also been invited to conduct a special session on the nature of cognitive flexibility in educational practices to student teachers as part of NIE's Office of Teacher Education's organisation of the "Teachers as Thinkers (TaT)" series (September 2024). The talk will feature how neuroscience, social science, and other areas of research have important implications on education, and how it can be addressed by educators through designing conducive learning environments and practicing innovative pedagogy in classrooms.

The School Workgroup have hosted several activities to improve adolescents' engagement in activities promoting and assessing Cognitive Flexibility via brain-based games (i.e., earthquake challenge, grid game, CF tasks, etc.) at the Inaugural Kids' Conference Asia in Singapore on 9 July 2024, an initiative by the Knowledge Building Community at NIE.

View the Brainiverse artbook, *Neurodiversity: No Brain is the Same* online here: https://www.cares.cam.ac.uk/research/clic/

AMPLE

AN ACCELERATED MANUFACTURING PLATFORM FOR ENGINEERED NANOMATERIALS

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

Principal Investigator:

Professor Alexei LAPKIN
University of Cambridge

Project Lead:

Dr Nicholas JOSE
CARES

Since our last update in March 2024, AMPLE has had incredible progress, resulting in key technical and commercial developments. The team has also undergone changes, as **Mr Karim BEN HICHAM (Research Assistant, CARES)** departed at the end of his internship, and **Mr Thirunavukkarasu SELVARAJ (Process Technician)** and **Mr Jeremy LIM (Pilot Lab Technician)** joining. **Ms Kylie CHUA (Operations Manager, CARES)** has also taken on a new role as Operations Manager within the team to manage trial activities and business development operations on a full time basis.

As mentioned in our last progress report, AMPLE is developing unique, structured nano zinc oxide materials with high performance in coatings. Following the successful scale-up of the process to the multi-kilo per day scale with our K10 reactor, we have successfully completed trials in our K100 (100kg/day) reactor within CARES' pilot room. The team worked through a range of issues and automated system improvements to create a safe and fully automated system to run. The next stage of system testing is at a partner facility, Elite Advanced Materials in Malaysia, where the

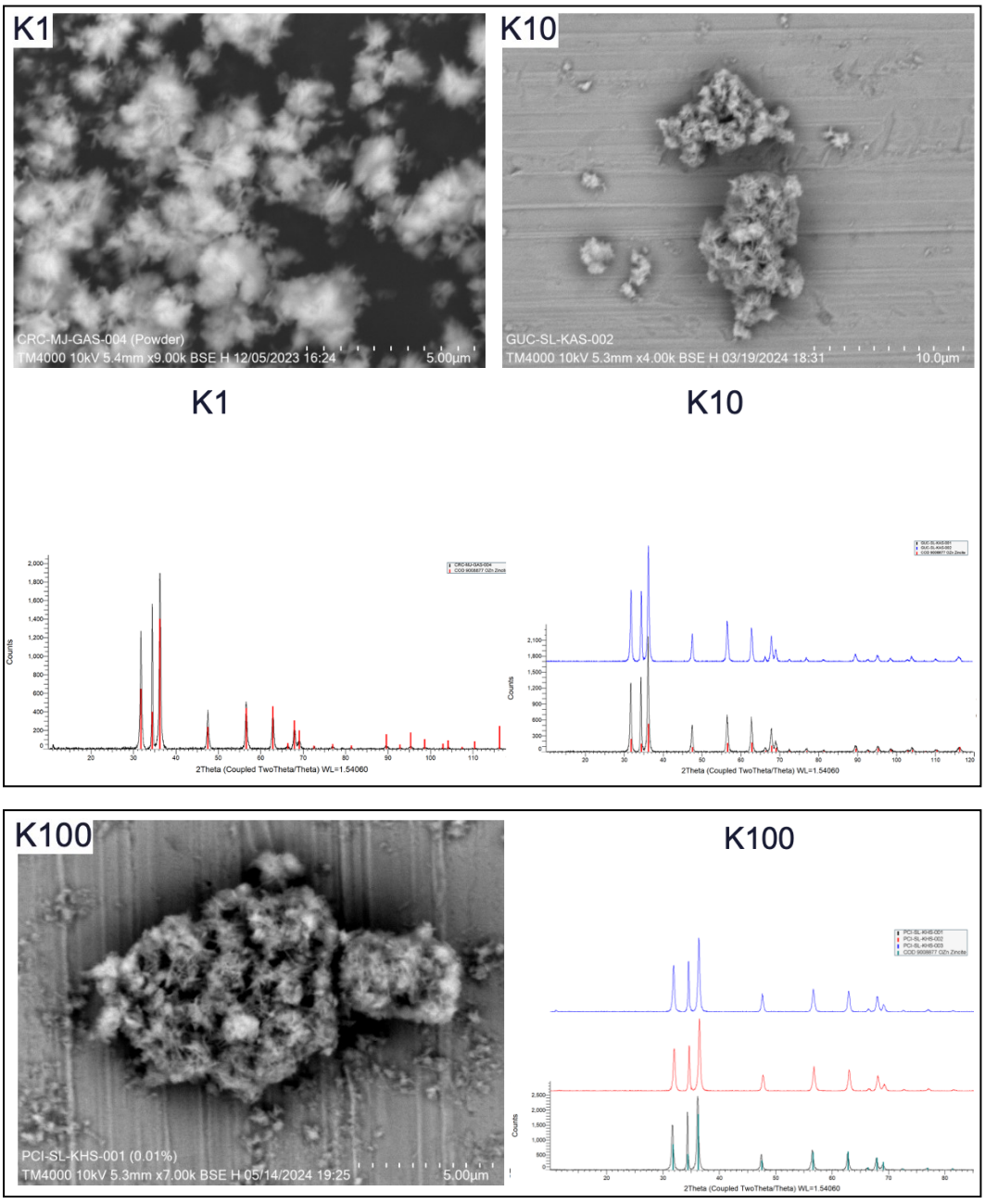


Figure 7.1: Scanning electron microscopy images and X ray diffraction patterns of ZnO synthesised across the K1, K10 and K100, indicating preservation of morphology and crystallinity.

system will run continuously for extended periods of time. This phase of the project will be delivered in October – November.

Launch of K1 Reactor System

Over the last six months, the AMPLE "K1" team has been hard at work developing the first commercial launch of the 1 kg/day reactor system for nanoparticle synthesis, creating a sleek, functional user interface. To date, the team has now successfully hosted three user trials with industrial R&D teams in Singapore. They have also synthesised three novel "proof-of-concept" samples for material producers across Japan, Singapore and the United States. The new system significantly reduces the footprint required to get people started, and conveniently fits inside a standard fume hood or bench.

The K1 Start

Our business development team has been promoting the system, highlighting its benefits in synthesis quality, performance, and cost efficiency. A significant pipeline of industrial users has been built up for those interested in using the K1, K10 and K100 series reactors.

Watch a promotional video on the system here: https://youtu.be/u6iHoC2UzG8

Fundraising/Spin-off

The team is now in late stage due diligence with investors to secure spin-off funding for the next two years of operations, aiming to close the round by the end of the year. The team plans to continue operations in Singapore for reactor construction and calibration, utilising shared lab space in Singapore for demonstrations and collaborations.

Figure 7.2: A screenshot of the K1 Reactor system from AMPLE's promotional video.

Other activities and achievements

AMPLE exhibited a booth at various events:

- ACHEMA in Frankfurt, Germany from 10 - 14 June 2024.
- FutureLabs in Basel, Switzerland from 25 - 27 June 2024.
- Advanced Innovation and Manufacturing Week in Penang, Malaysia from 3 - 4 September 2024.
- Pharma Pro&Pack in Hyderabad, India from 26 - 28 September 2024.

Dr Mikhail KOVALEV (Technical Development Manager) and **Dr Mohammed JERAAL (Materials Engineer, AMPLE)** both delivered oral presentations at Advanced Innovation and Manufacturing Week in Penang, Malaysia from 4 - 5 September 2024. These were "How to control properties and rapid scale-up of nanomaterials" and "Introduction to Accelerated Materials" respectively.

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

The following are the ongoing collaborations:

1. Suppliers: Vapourtec (UK)
2. End-users: Evonik (SG/GER), Pfizer (USA), KCTech (KR) NXMaterials (KR), Estee Lauder (USA), Nanolumi (SG)
3. Distributors: Automed (IN), Kowa (SG/JP), Ehrfeld Microteknik (GER)

Accelerated Materials, AMPLE's registered company in Singapore, is part of the Top 50 Global finalists of Singapore's "SLINGSHOT" pitching competition, taking place in October. The top 3 prizes comes with a startup grant and rent-free space at a co-working location in Singapore.

PIPS

PHARMA INNOVATION PROGRAMME SINGAPORE

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

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

CARES Principal Investigators:

Professor Markus KRAFT
University of Cambridge

Professor Alexei LAPKIN
University of Cambridge

Automated Evaluation of Environmental Impacts of Pharma Manufacturing Processes

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

Automated Evaluation of Environmental Impacts of Pharma Manufacturing Processes is a three-year project that started in July 2023 funded by the Pharma Innovation Programme (PIPS 2) programme and led by **Prof Alexei LAPKIN (CAM)**.

CARES has sub-contracted the research and development work on this project to its spin-off company Chemical Data Intelligence (CDI) Pte Ltd. CDI works with proprietary data, is set-up to productise software for application in the chemical industry.

During the period covered in this report, the project team has expanded, involving new industry partner, Boehringer Ingelheim, and also including a PhD student and a post-doc from the University of Cambridge. The team expansion allows the overall project to progress faster in several of its sub-challenges. In this period, the project team has delivered the first demo of one of the workflows towards automated generation of life cycle impacts.

From Digital Twins to Real Time AI-supported Plant Operation

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

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

CARES' contribution to this project involves two main aspects: developing a generic formulation of physical models for processes (performed by the modelling team) and developing and/or extending existing process ontologies to instantiate ontology-based digital twins in the knowledge graph (performed by the ontology team). In this project, CARES also collaborates closely with the A*STAR Institute for Infocomm Research (I^2R), hereinafter referred to as the implementation team, to build and implement the digital infrastructure for the selected process. After numerous discussions and considering the project's ease of access, the Accelerated Manufacturing Platform for Engineered Nanomaterials (AMPLE) plant was selected to demonstrate the workflow developed within our project. (Read more about AMPLE on page 78).

During this reporting period, the modelling team developed an ontology-based digital twin framework for maintaining physical models in chemical processes, as illustrated in Figure 8.1. Beginning with process information collection, the developed knowledge graph can assemble solvable equations into a physical model. Following parameter fitting, the derived model can be applied to downstream tasks, such as process prognostics, product prediction, and process optimisation. To ensure the model's continued applicability, a model maintenance module is incorporated to update the process information and physical model.

A case study applying the ontology-based digital twin method was developed using an annular microreactor, as shown in Figure 8.2. In the annular microreactor, engulfment mixing is identified as the primary mixing mechanism for streams, sheared by the gas flow in the tube. The Villermaux-Dushman reaction system was employed to characterise the micromixing efficiency. Fol-

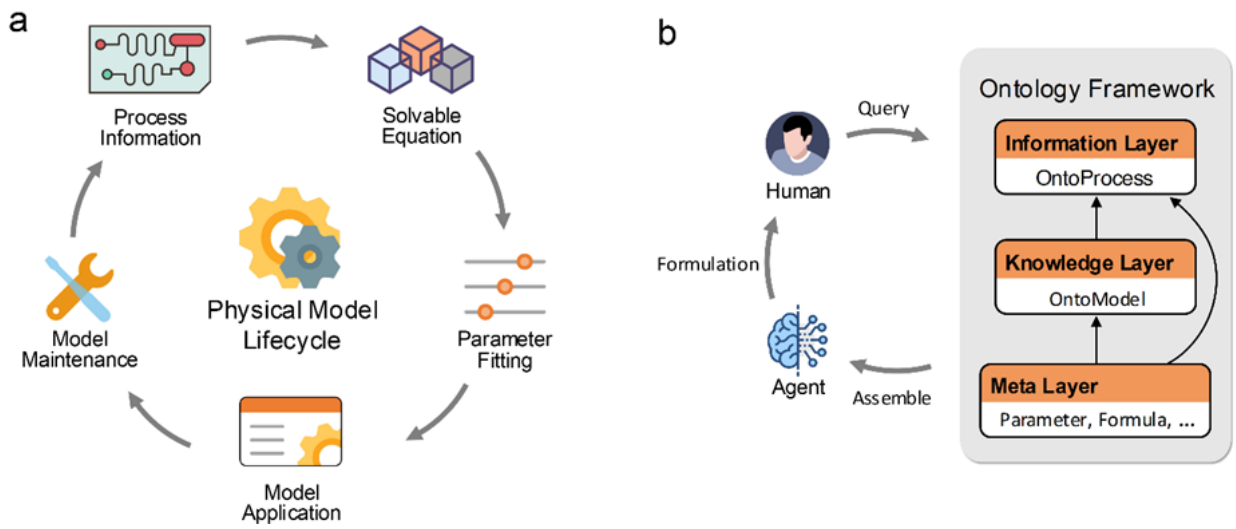


Figure 8.1: (a) The lifecycle of a physical model built using a knowledge graph. Each arrow represents a software agent. (b) Generic ontological framework for handling physical models through human-software interaction.

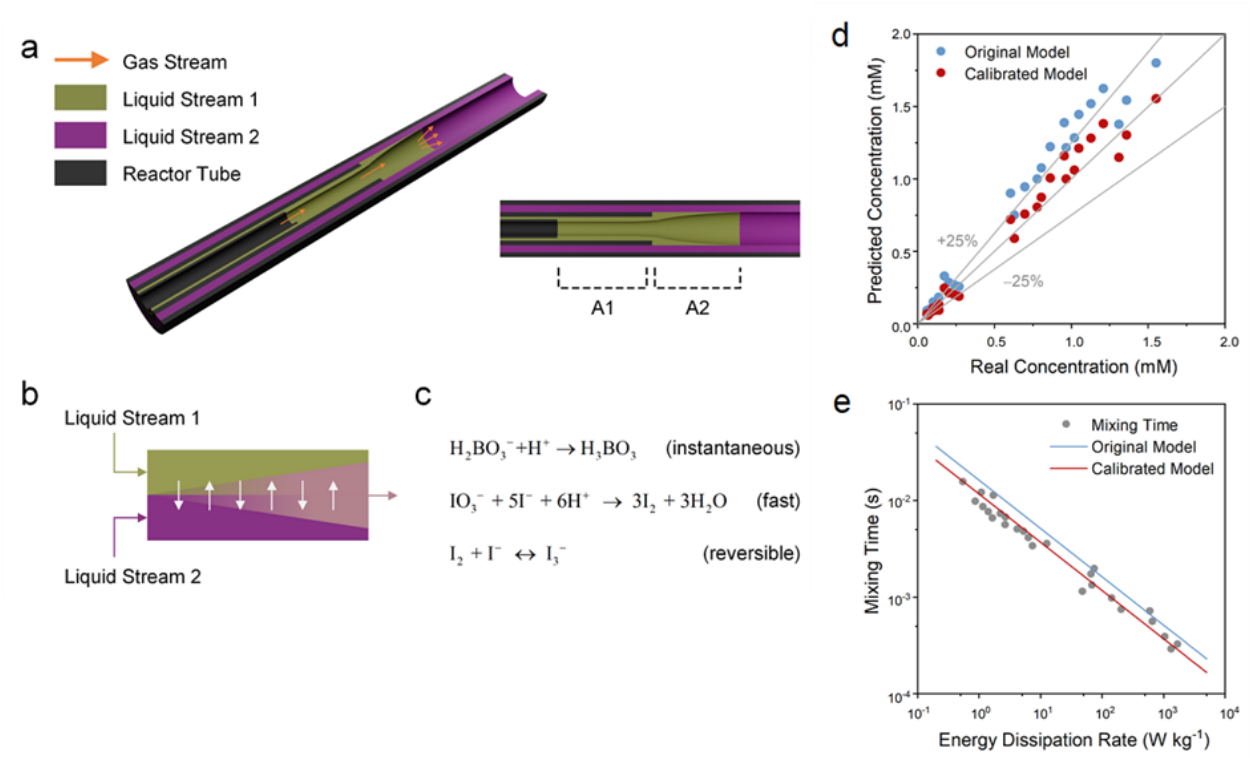


Figure 8.2: Application of the ontology-based digital twin method to the annular microreactor. (a) Structure of the plug flow annular microreactor. (b) Illustration of engulfment mixing. (c) Villermaux-Dushman reaction system. (d) Parity plots of predicted and real I_3^- concentrations for the original and calibrated models. (e) Relationships between mixing time and energy dissipation rate.

lowing model calibration, the predicted concentration of I_3^- matched the measurements over a broad range. The relationship between mixing time and energy dissipation rate was also calibrated to ensure the model's applicability.

The ontology team completed the development and extension of ontologies to represent selected devices, their associated parameters, and data within the knowledge graph for all modules in AMPLE's pilot plant, including the Dosing, Reactor, and Purification modules. These ontologies were developed based on the plant's process flow diagram and Kepware's Open Platform Communications Unified Architecture (OPC-UA) server variables provided by the AMPLE team, utilising existing ontologies such as the Financial Industry Business Ontology (FIBO), OntoDevice (an ontology for describing devices and their properties), OntoBMS (an ontology for describing Building Management Systems), OntoCAPE (an ontology for the domain of Computer-Aided Process Engineering), the Ontology of Measure, SAREF (an ontology for describing smart devices and applications), and s4bldg (a SAREF extension for describing buildings). Figure 8.3 provides a visual representation of the ontology developed for the Purification module.

The ontology team also worked closely with the I²R team and AMPLE to develop a data streaming architecture and its associated agents to connect AMPLE's Kepware OPC-UA server to the I²R edge device, as depicted in Figure 8.4. Security features have been integrated into this architecture through the use of Nginx and Keycloak.

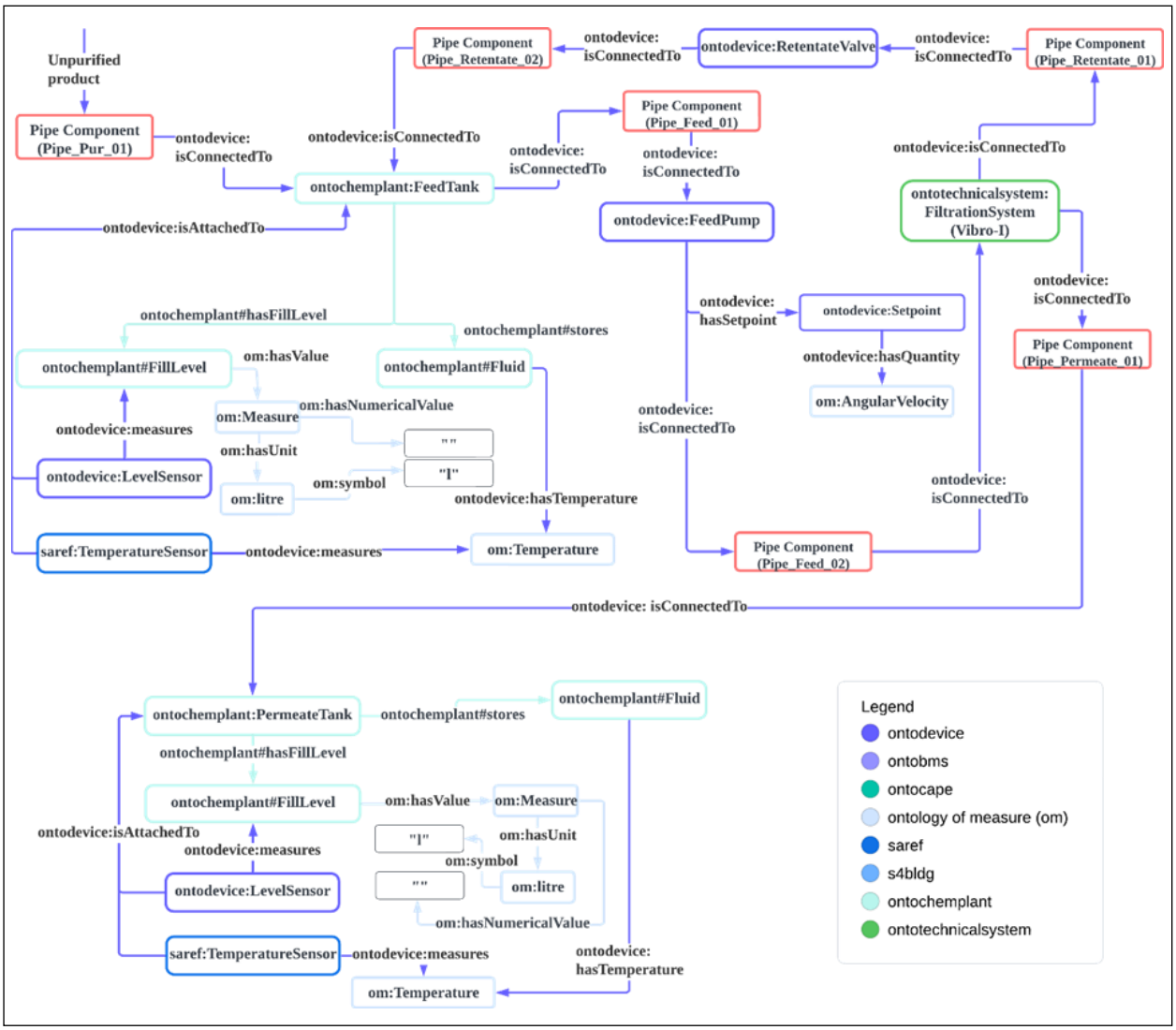


Figure 8.3: A snippet of the ontology for the Purification module of AMPLE's pilot plant. The details of the 'Pipe Component' ontology and some aspects of the Ontology of Measure are not included due to space constraints.

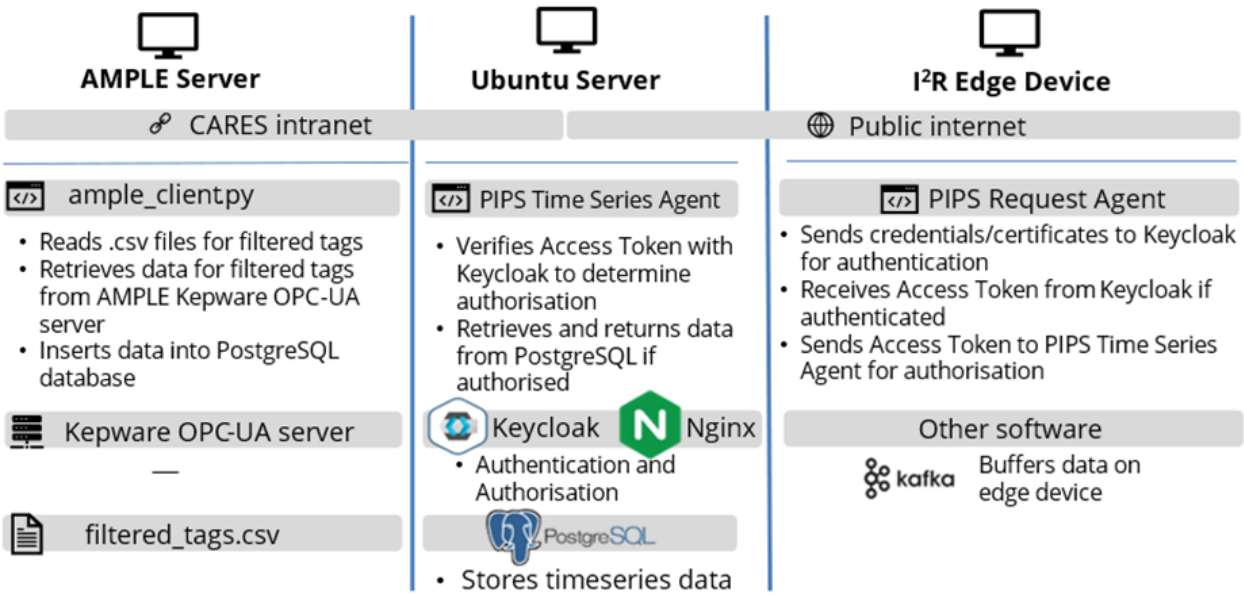


Figure 8.4: Data streaming architecture for connecting AMPLE's Kepware OPC-UA server to the I²R edge device.

Dr Dogancan KARAN (Research Fellow, CARES) has continued work on predicting the life cycle impact of waste water treatment processes in pharmaceutical companies through mechanistic and data-driven models. This involves collecting time series data of different unit operations (separation and waste water treatment units from various industrial manufacturing sides), cleaning and populating the data, and finally building different various models around the data for the prediction of the life cycle impact. Dr Karan has completed one case study for predicting the lifecycle inventory of non-biological aqueous waste water treatment process. A machine learning model has been trained on 2 years-worth of historical process data. The model accepts the waste amount (m^3), waste temperature (^oC), and pH and predicts 5 different utilities to treat the waste—electricity consumption (kW), acid/base consumption (L), cooling duty (kW) and chilling duty (kW).

OTHER PROJECTS

OTHER CARES-FUNDED PROJECTS

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

The current CARES small projects include a contribution towards Cooling Singapore 2.0 hosted by the Singapore-ETH Centre, and two projects in the Low-Carbon Energy Research (LCER) Phase 2 Programme, one hosted by NUS and one hosted by NTU.

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

Cooling Singapore 2.0

In collaboration with the Singapore-ETH Centre

Cooling Singapore 2.0 aims to construct a Digital Urban Climate Twin (DUCT) for Singapore. This platform integrates several computational models (environmental, land surface, industrial, traffic, building, and energy) and climate models to investigate ways to reduce Singapore's urban heat and mitigate its effects. In addition, the DUCT will allow researchers to trial various scenarios and predict their impact on urban heating.

CARES' contribution to Cooling Singapore 2.0 is to estimate anthropogenic heat emissions from industrial activity in Singapore by developing computational energy models using The World Avatar (TWA). The results of these models constitute the input for the DUCT.

During this reporting period, City Energy Analyst (CEA) simulations were performed for eight data centre buildings in Singapore. These simulations were based on energy usage estimations obtained from the literature and were aimed at developing representative characteristics for estimating energy consumption of data centres within the CEA. As part of this effort, five parameters specific to data centres have been implemented as configurable parameters associated with building types, allowing users to adjust these values as needed. The five parameters are:

- The temperature at which refrigerant is supplied to the servers,
- The temperature at which refrigerant is returned from the servers,
- The efficiency of the heat pump,
- The ratio of electrical energy used by the compressor to the total energy used by the cooling system, and
- The fraction of electrical energy supplied to servers that is emitted as heat.

Additionally, two new industry types (semiconductor and pharmaceutical) have been incorporated into the CEA module within the DUCT to estimate their respective energy consumption. As illustrated in Figure 9.1, for the same building, setting the building usage to 'semiconductor' results in an annual electricity consumption of 465,404 MWh, whereas setting the building usage to 'pharmaceutical' results in a higher annual electricity consumption of 598,180 MWh.

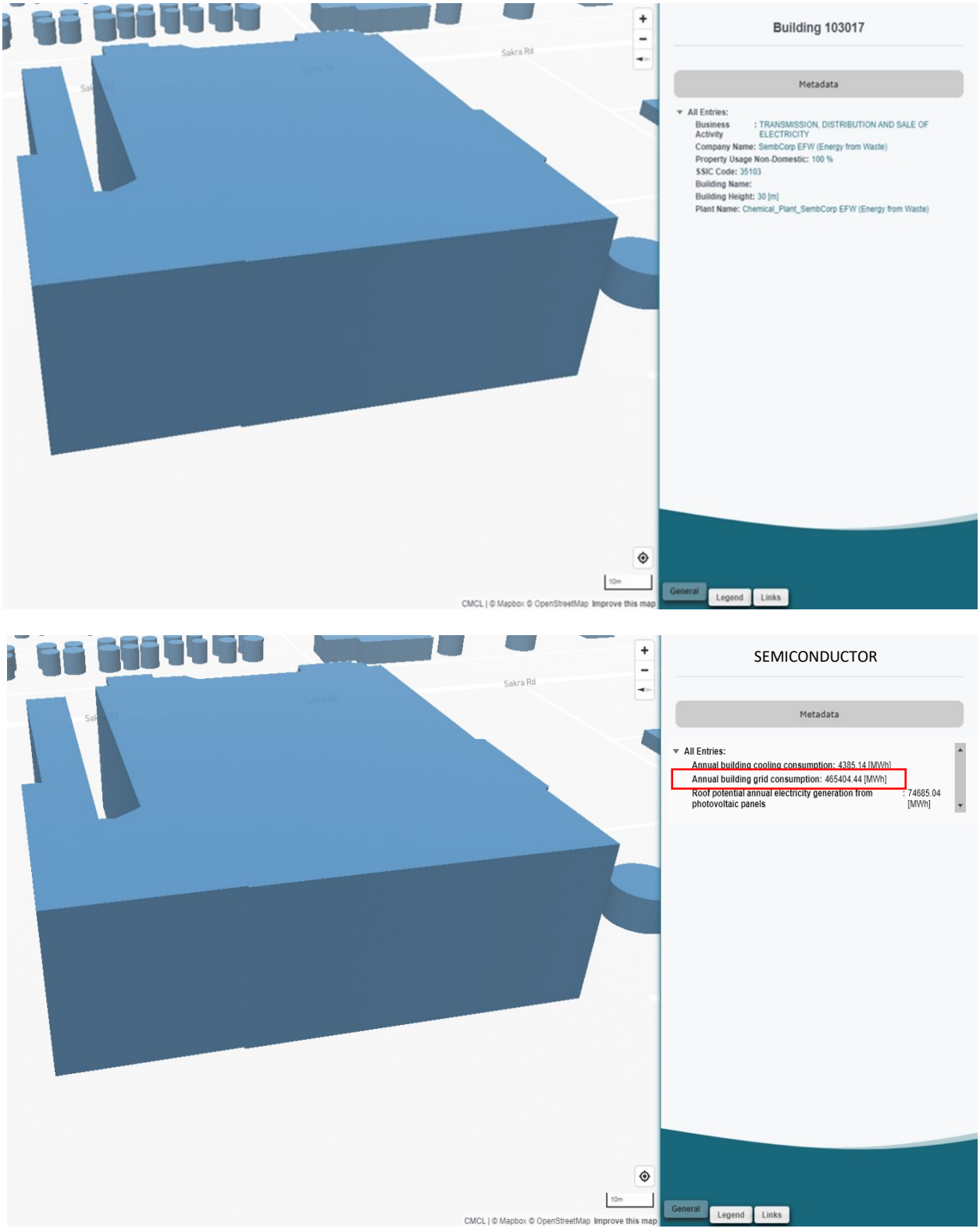


Figure 9.1: City Energy Analyst (CEA) simulation results for a building providing an estimation of its annual electricity consumption as well as its potential for rooftop photovoltaic energy generation. Setting the building usage to 'semiconductor' or 'pharmaceutical' yields different grid consumption outcomes, as highlighted by the red rectangles.

Low-Carbon Energy Research Phase 2

In collaboration with the National University of Singapore

Dr B HARIKRISHNAN (Research Fellow, CARES) has been actively engaged in the LCER project, which focuses on the numerical investigation and validating of the **LES-CMC** solver for the experiment for the SINTEF sequential combustor for ammonia (Figure 9.2, Ditaranto and Saanum, 2024; DOI: 10.1016/j.combustflame.2024.113368). Initial steps involved progressively simulating Reynolds Average Navier-Stokes (RANS) and Large Eddy Simulation (LES) to understand the cold flow. This approach primarily aids in visualising the mixing field, which serves as a foundation for initialising combustion simulations.

The project's primary objective is to develop a reduced order model, referred to as the Incompletely Stirred Reactor Network (ISRN), to explore the design space of the ammonia gas turbine under varying conditions, including pressure (P), fuel/air temperature (T), primary zone equivalence ratio (Φ_{z1}), and ammonia decomposition ratio (DR). Figure 9.3 illustrates the relationship between DR and species volume fractions, while Figure 9.4 provides an overview of the research plan.

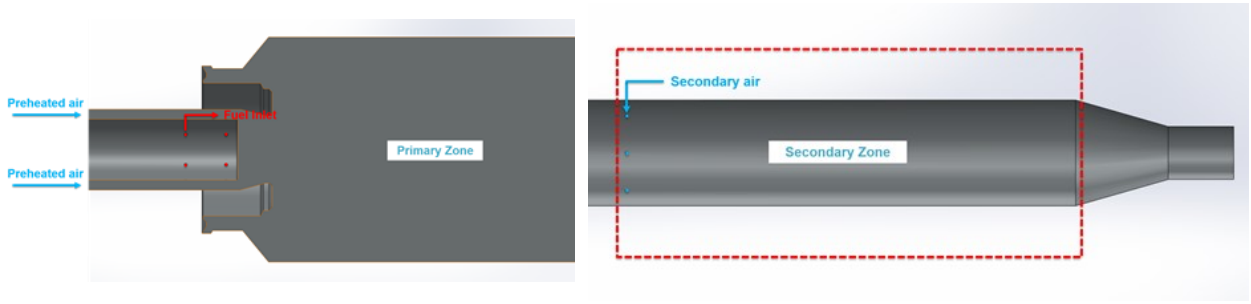


Figure 9.2: Primary and secondary zone of the SINTEF sequential combustor.

Dr B HARIKRISHNAN

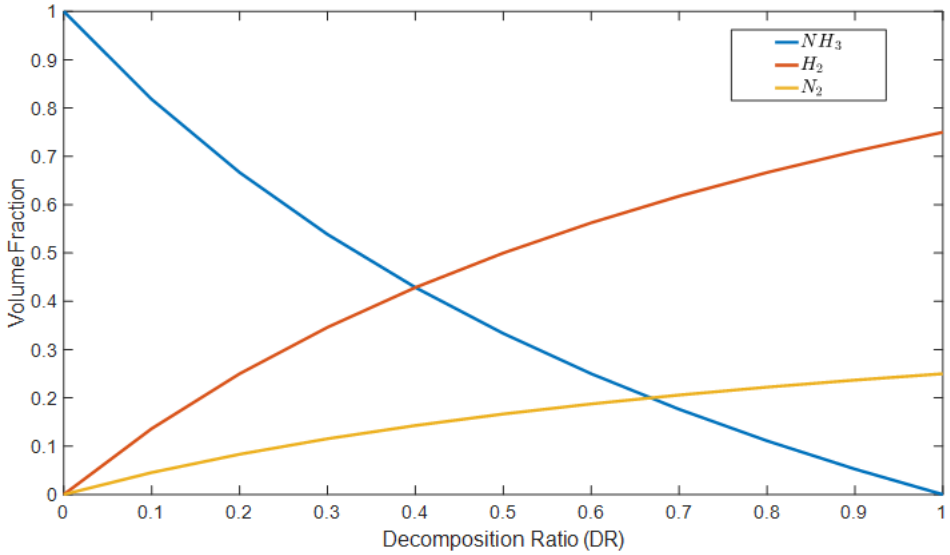


Figure 9.3: Volume fraction of fuel species (NH_3/H_2/N_2) vs decomposition ratio (DR).

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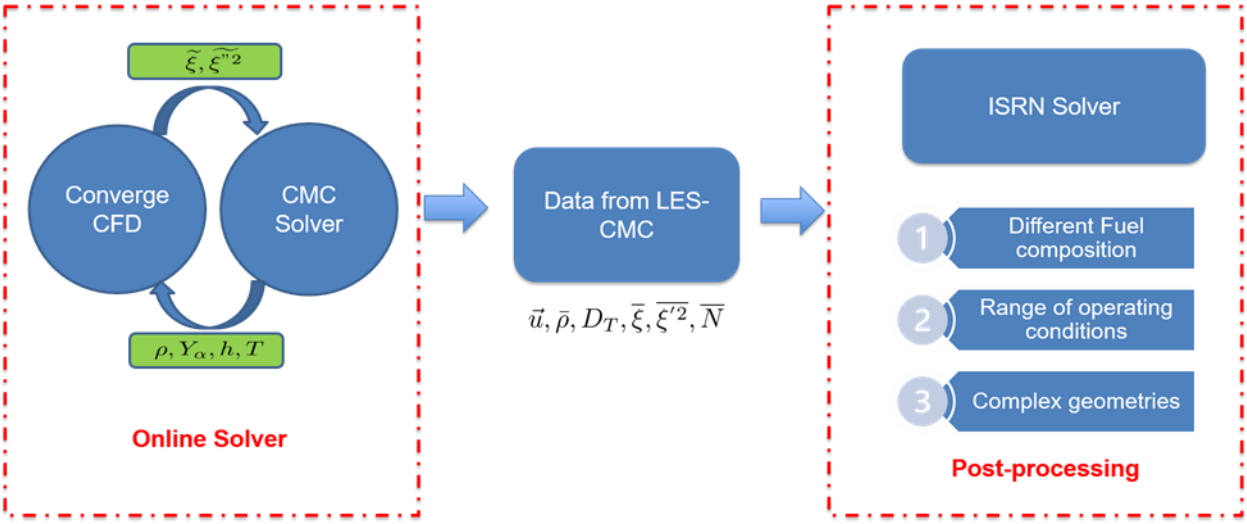

Figure 9.4: Research plan for the SINTEF combustor.

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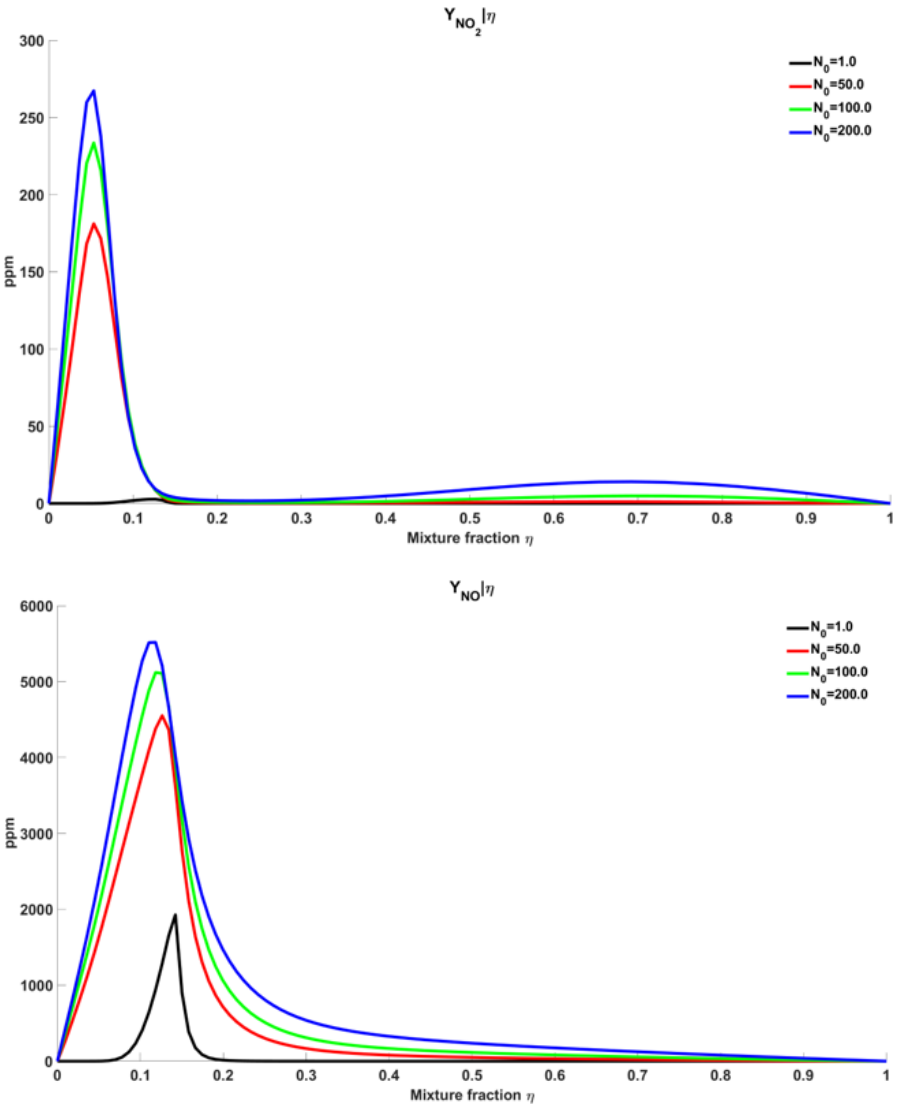

Figure 9.5: Conditional expectation of NOx obtained using 0D-CMC for different prescribed scalar dissipation rate (DR=0.25).

Dr B HARIKRISHNAN

Detailed 0D-CMC simulations are being conducted to assess different combinations of P, T, and DR values. These simulations are critical for building a priori understanding of how the scalar dissipation rate (SDR), alongside operating conditions and fuel options, impacts the conditional expectation of reactive species, particularly NOx and N_2O (Figures 9.5-9.7).

Figures 9.8 and 9.9 display the mixing field (mixture fraction ξ) and the scalar dissipation rate (N). Preliminary 0D-CMC simulations suggest that elevated SDR near the burner exit leads to high emissions in this region.

Currently, the researcher is conducting LES-CMC simulations to further investigate the mixing field. Key statistics are being collected from these simulations, which will subsequently be used to initiate the post-processing phase, i.e., ISRN solver

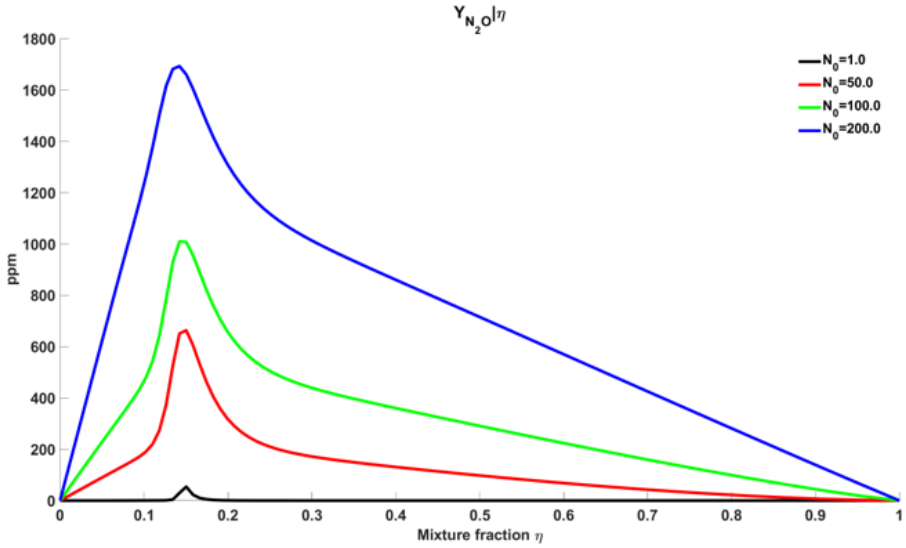

Figure 9.6: Conditional expectation of N_2O obtained using 0D-CMC for different prescribed scalar dissipation rate (DR=0.25).

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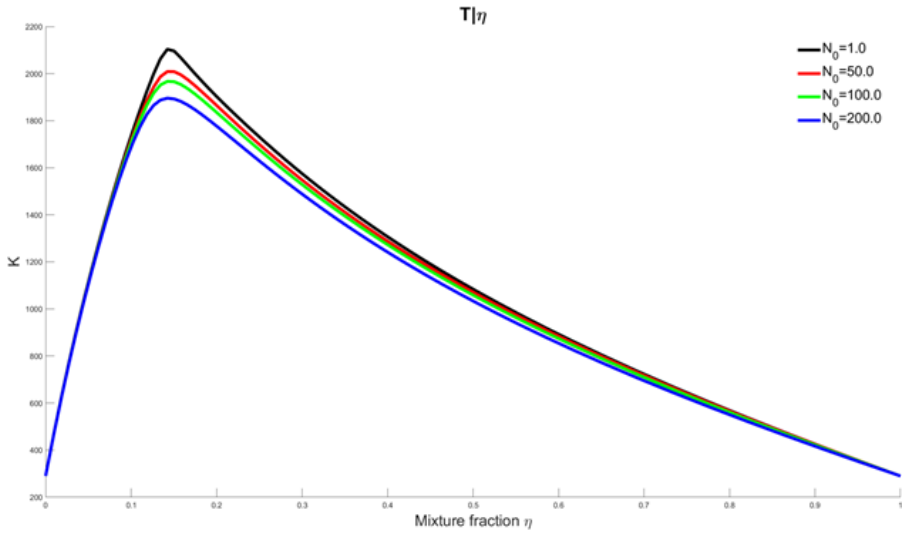

Figure 9.7: Conditional expectation of temperature T obtained using 0D-CMC for different prescribed scalar dissipation rate (DR=0.25).

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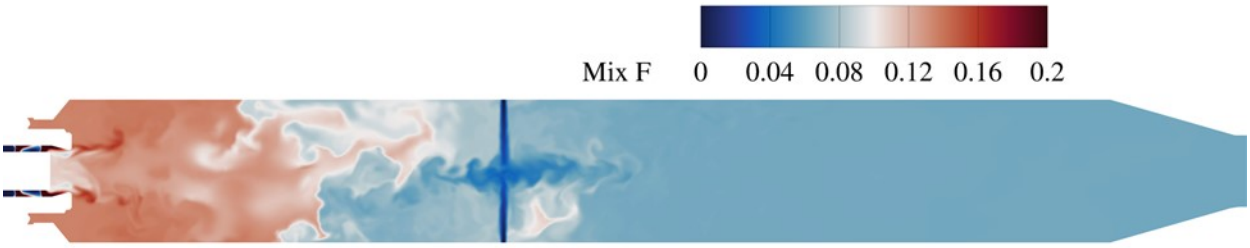

Figure 9.8: Mixture fraction field for $T_{air} = T_{fuel} = 576.15\,K$, $P = 10$ *bar and primary zone equivalence ratio* $\phi_{z1} = 1.0$.

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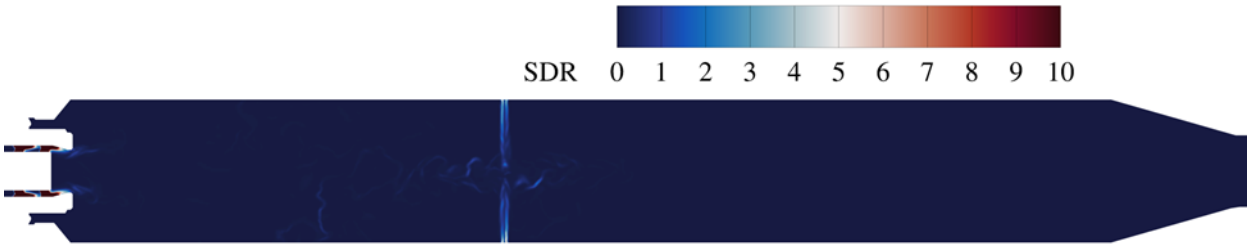

Figure 9.9: Scalar dissipation rate for $T_{air} = T_{fuel} = 576.15\,K$, $P = 10$ *bar and primary zone equivalence ratio* $\phi_{z1} = 1.0$.

Dr B HARIKRISHNAN

PUBLICATIONS

ALL C4T PUBLICATIONS WITH CREATE ACKNOWLEDGEMENT

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

C4T impact-focused "CN" projects

- Bai, Jiaru, Kok Foong Lee, Markus Hofmeister, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft. 2024. 'A Derived Information Framework for a Dynamic Knowledge Graph and Its Application to Smart Cities'. *Future Generation Computer Systems* 152 (March):112–26. https://doi.org/10.1016/j.future.2023.10.008.
- Bai, Jiaru, Sebastian Mosbach, Connor J. Taylor, Dogancan Karan, Kok Foong Lee, Simon D. Rihm, Jethro Akroyd, Alexei A. Lapkin, and Markus Kraft. 2024. 'A Dynamic Knowledge Graph Approach to Distributed Self-Driving Laboratories'. *Nature Communications* 15 (1): 462. https://doi.org/10.1038/s41467-023-44599-9.
- Chen, Yubo, Daniel J. Zheng, Zhichuan J. Xu, and Yang Shao-Horn. 2024. 'Best Practices for Oxygen Electrocatalysis'. *Nature Sustainability*, February. https://doi.org/10.1038/s41893-024-01285-y.
- **Chin Law, Li, Savvas Gkantonas, Agustin Mengoni, and Epaminondas Mastorakos. 2024. 'Onboard Pre-Combustion Carbon Capture with Combined-Cycle Gas Turbine Power Plant Architectures for LNG-Fuelled Ship Propulsion'. *Applied Thermal Engineering* 248 (July):123294. https://doi.org/10.1016/j.applthermaleng.2024.123294.**
- Chitre, Aniket, Jayce Cheng, Sarfaraz Ahamed, Robert C. M. Querimit, Benchuan Zhu, Ke Wang, Long Wang, Kedar Hippalgaonkar, and Alexei A. Lapkin. 2024. 'PHbot: Self-Driven Robot for PH Adjustment of Viscous Formulations via Physics-informed-ML**'. *Chemistry–Methods* 4 (2): e202300043. https://doi.org/10.1002/cmtd.202300043.
- **Chitre, Aniket, Robert C. M. Querimit, Simon D. Rihm, Dogancan Karan, Benchuan Zhu, Ke Wang, Long Wang, Kedar Hippalgaonkar, and Alexei A. Lapkin. 2024. 'Accelerating Formulation Design via Machine Learning: Generating a High-Throughput Shampoo Formulations Dataset'. *Scientific Data* 11 (1): 728. https://doi.org/10.1038/s41597-024-03573-w.**

- **Dai, Chencheng, Qian Wu, Tianze Wu, Yuwei Zhang, Libo Sun, Xin Wang, Adrian C. Fisher, and Zhichuan J. Xu. 2024. 'Suppressing Product Crossover and C–C Bond Cleavage in a Glycerol Membrane Electrode Assembly Reformer'. *Energy & Environmental Science* 17 (17): 6350–59. https://doi.org/10.1039/D4EE01824A.**
- **Eibeck, Andreas, Shaocong Zhang, Mei Qi Lim, and Markus Kraft. 2024. 'A Simple and Efficient Approach to Unsupervised Instance Matching and Its Application to Linked Data of Power Plants'. *Journal of Web Semantics* 80 (April):100815. https://doi.org/10.1016/j.websem.2024.100815.**
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- **Hofmeister, Markus, Jiaru Bai, George Brownbridge, Sebastian Mosbach, Kok F. Lee, Feroz Farazi, Michael Hillman, et al. 2024. 'Semantic Agent Framework for Automated Flood Assessment Using Dynamic Knowledge Graphs'. *Data-Centric Engineering* 5:e14. https://doi.org/10.1017/dce.2024.11.**
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- **Hofmeister, Markus, Kok Foong Lee, Yi-Kai Tsai, Magnus Müller, Karthik Nagarajan, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft. 2024. 'Dynamic Control of District Heating Networks with Integrated Emission Modelling: A Dynamic Knowledge Graph Approach'. *Energy and AI* 17 (September):100376. https://doi.org/10.1016/j.egyai.2024.100376.**
- **Jelinek, Thorsten, Amit Bhave, Nicolas Buchoud, Michael Max Bühler, Patrick Glauner, Oliver Inderwildi, Markus Kraft, Charles Mok, Konrad Nübel, and Axel Voss. 2024. 'International Collaboration: Mainstreaming Artificial Intelligence and Cyberphysical Systems for Carbon Neutrality'. *IEEE Transactions on Industrial Cyber-Physical Systems* 2:26–34. https://doi.org/10.1109/TICPS.2024.3351624.**
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