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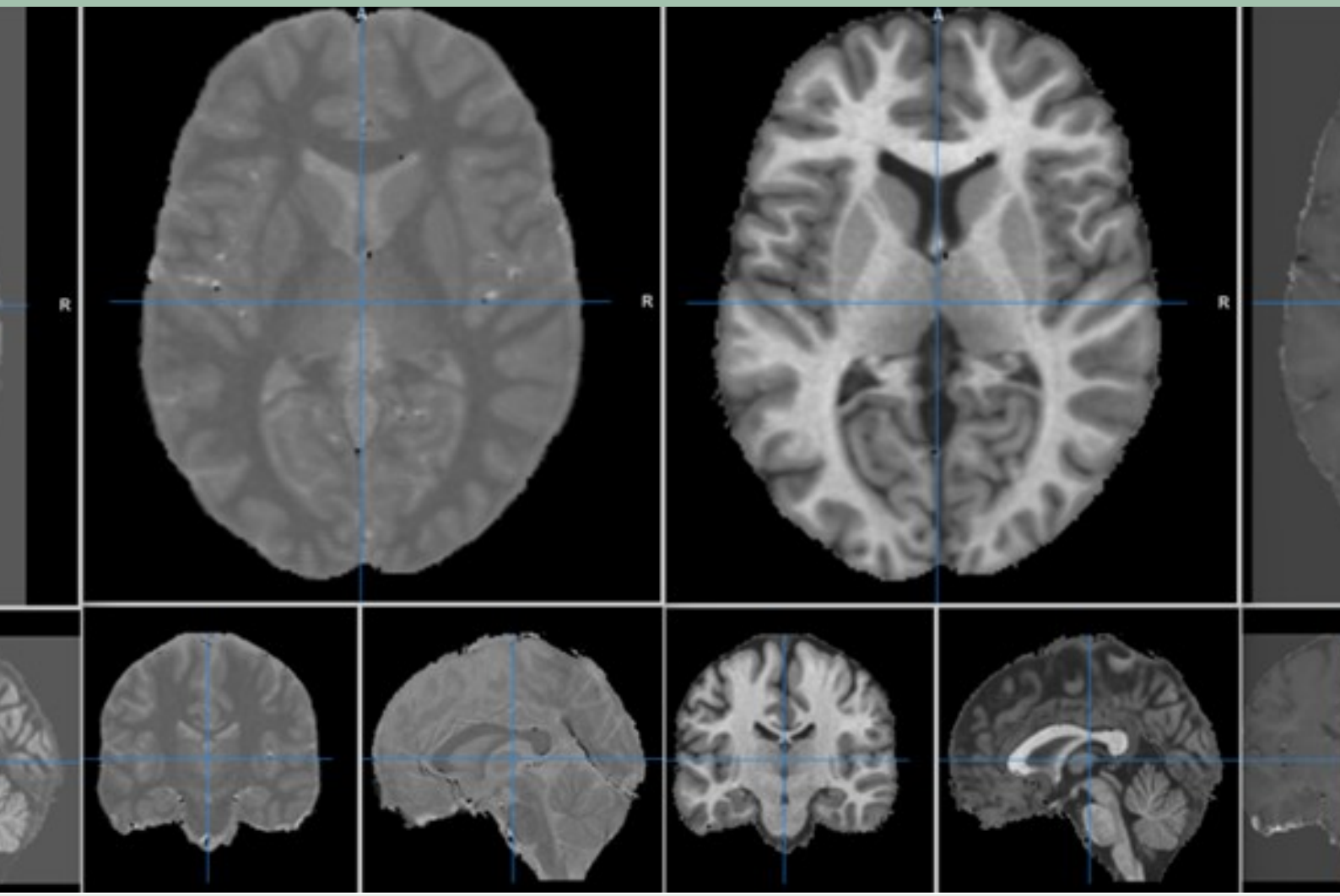
A COLLABORATION BETWEEN THE UNIVERSITY OF CAMBRIDGE,
NANYANG TECHNOLOGICAL UNIVERSITY & NATIONAL UNIVERSITY OF SINGAPORE



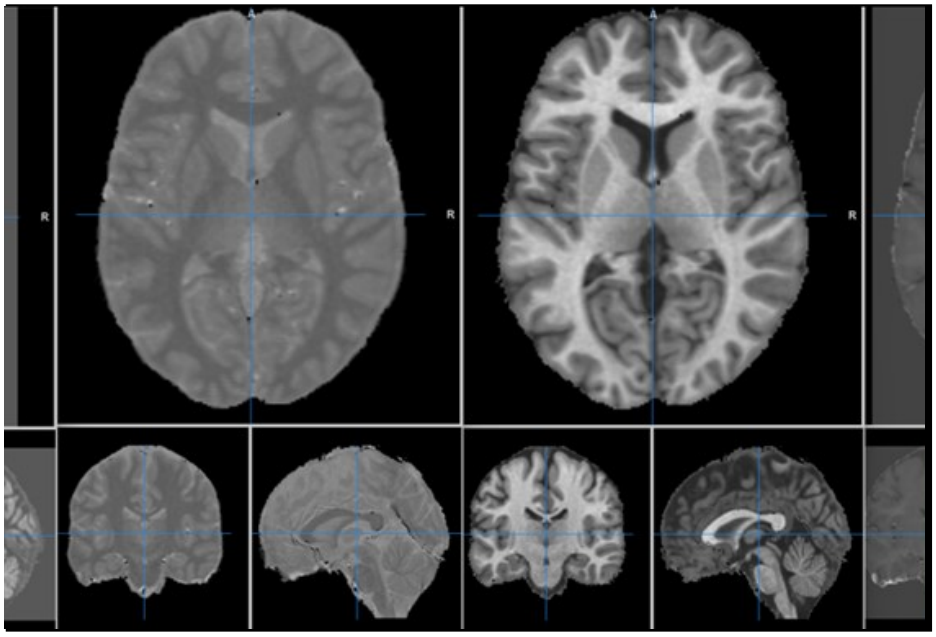
Biannual Research Report

October 2023 - March 2024

CAMBRIDGE
CARES

CAMBRIDGE CENTRE
FOR ADVANCED RESEARCH AND
EDUCATION IN SINGAPORE LTD

Cover image



An illustrative example of CLIC's multi-parametric maps data and processed maps generated for further region of interest (ROI) and group-based data analysis. These maps relate to microstructural neuronal changes as a measure of the myelination process in white matter believed to be modulated by learning and adaptation to novel experiences.

Image by the CLIC Neuroimaging Workgroup. *See more on page 77.*

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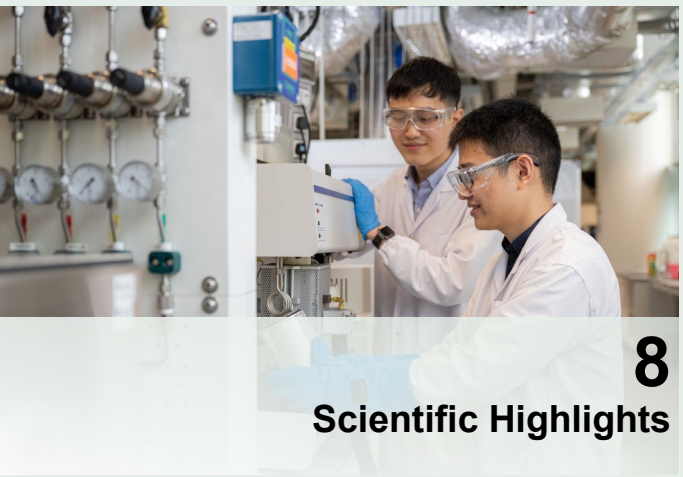
1 Create Way, #05-05 CREATE Tower
Singapore, 138602

enquiries@cares.cam.ac.uk
www.cares.cam.ac.uk



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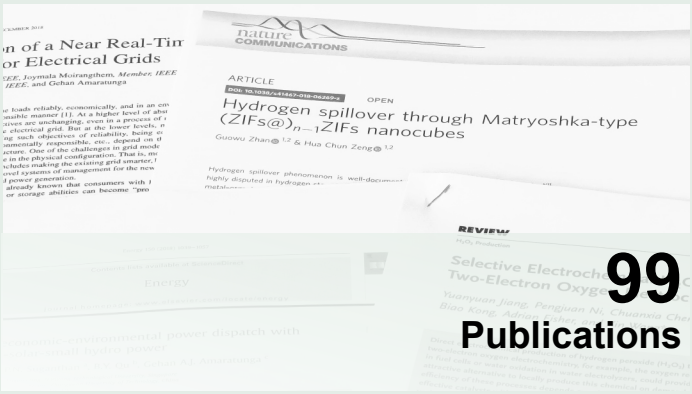

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FOREWORD

Our UK and Singapore teams celebrated CARES' 10th Anniversary on 1st December 2023 with a Scientific Showcase and an evening reception hosted by the British High Commission in Singapore. It was truly a commemorative day that showcased the best of our scientific impacts through four thematic sessions in the morning: Chemical Technologies and Processes, Digital Transformation, From Emissions to Solutions, and Lifelong Learning. The event transitioned neatly to a smaller evening session highlighting the importance of international research cooperation with a Distinguished Lecture speech by founding CARES board member, Prof Dame Lynn Gladden. In keeping with the theme of international partnerships, I am pleased that our Communications team in Singapore were able to work with their counterparts in the University of Cambridge to co-produce a video and story about CARES that is a terrific summary of our journey thus far. In addition, we also shortlisted "10 Scientific Images" from our research – all these materials are available here for your viewing: https://www.cares.cam.ac.uk/10anniversary/

C4T transitions to impact-focused projects

As we complete our first decade, we are delighted that the flagship Centre for Carbon Reduction in Chemical Technologies (C4T) programme that brought us to Singapore has been extended to enter a phase of impact-focused projects. There is stronger cross-over between our research teams and many projects are reaching a stage where there are discussion for industry partnerships and trials.

Spin-offs development

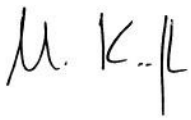
CARES has been able to initiate five active spin-offs in Singapore. Two were recently incorporated, demonstrating the maturity of technologies developed within C4T and the future pathways for some of our senior researchers. 3Y Energy has been accepted for the first phase of the SMART Innovation Grant 2.0 to support the launch of successful ventures, and EMICAST has been working with maritime industry specialists to refine their online calculator to improve ship optimisation and emissions forecasting. I anticipate great developments from our spin-offs.

CLIC researchers in Channel News Asia documentary

I enjoyed the recent Channel News Asia documentary "Nudge" which featured our Centre for Lifelong Learning and Individualised Cognition (CLIC) Social Workgroup on a segment discussing how simple changes to our environment can promote healthy eating. Although CLIC's Social aspect focuses on decision-making tendencies and mental flexibility rather than diet choices, it is exciting to see our research across these different disciplines.

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
March 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 recently 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

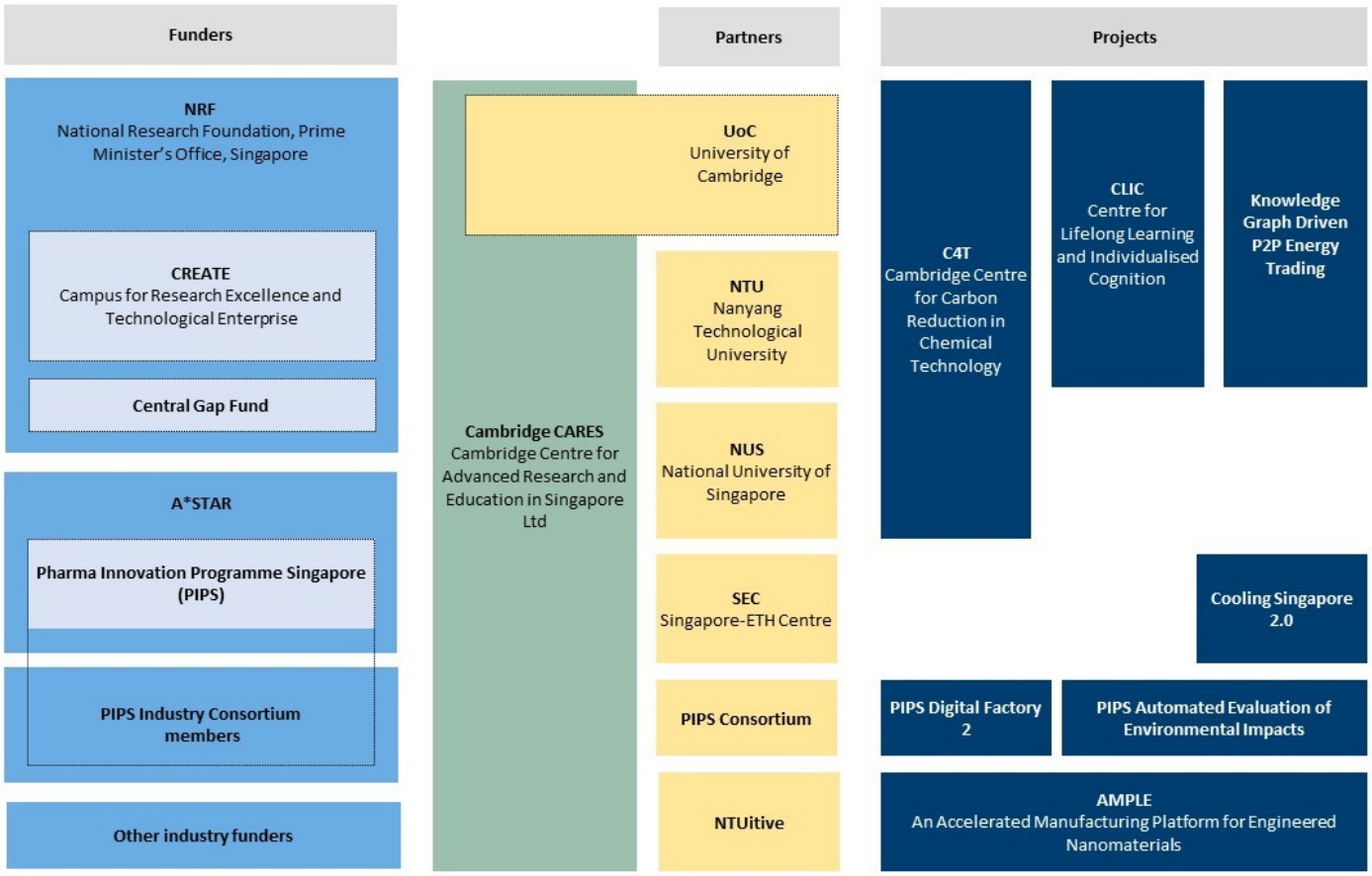
within the C4T programme and is currently looking to bring their products to commercialisation via the spin-off company Accelerated Materials.

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.

There are several other projects ongoing: The Intra-CREATE seed funded Knowledge Graph Driven P2P Energy Trading and Real-time Network Operation for High Renewables, and the CARES contribution in the Cooling Singapore 2.0 programme hosted by the Singapore-ETH Centre. Details and updates for these smaller projects can be found on page 93.

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 September 2023 - March 2024

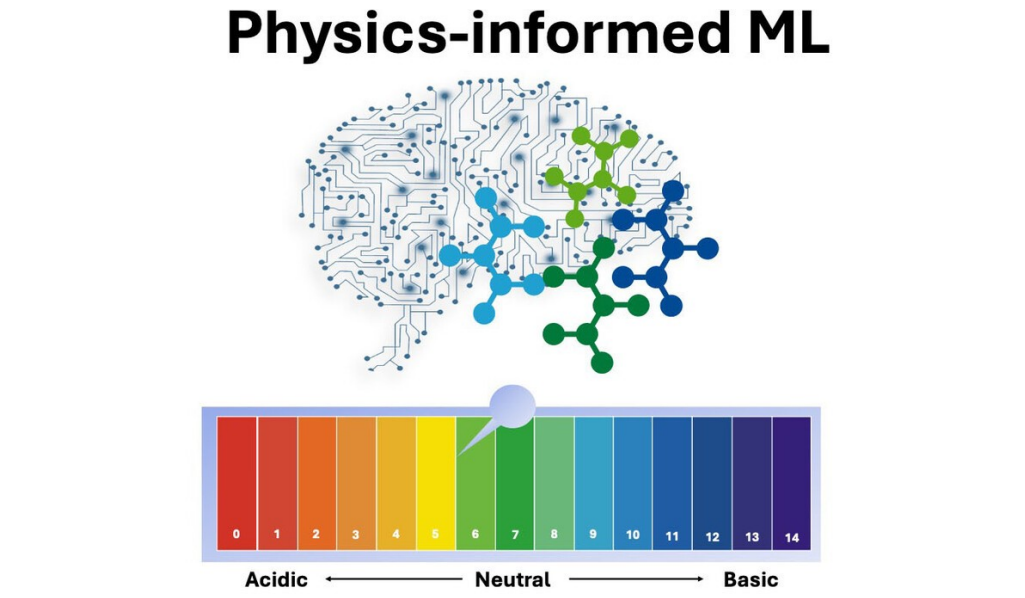
A selection of publications from across our programmes.

C4T: pHbot: Self-Driven Robot for pH Adjustment of Viscous Formulations via Physics-informed-ML

Aniket Chitre, Jayce Cheng, Sarfaraz Ahamed, Robert Querimit, Benchuan Zhu, Ke Wang, Long Wang, Kedar Hippalgaonkar, and Alexei Lapkin, *Chemistry-Methods*

DOI: 10.1002/cmtd.202300043

Abstract: pH adjustment is crucial for many industrial products, yet this step is typically performed by manual trial-and-error. A particularly industrially relevant yet challenging titration is that of adjusting viscous liquid formulations using weak, polyprotic titrants (usually citric acid). Handling of viscous, non-Newtonian formulations, with such polyprotic acids preferred for their chelation and buffering effects make a robotic solution challenging. We present a self-driving pH robot integrated with physics-informed learning; this hybrid physical-ML model enables automated titration with weak-strong acid/base pairs. To deal with the high viscosities of these formulations, we developed specific automated mixing and cleaning protocols. We hit the target pH within two to five iterations over 250 distinct formulations in lab-scale small-batch (~10 mL and 12 samples) titrations. In the interest of scaling up to match industrial processes, we also demonstrate that our hybrid algorithm works at ~25× scale-up. The method is general, and we open-source our algorithm and designs.

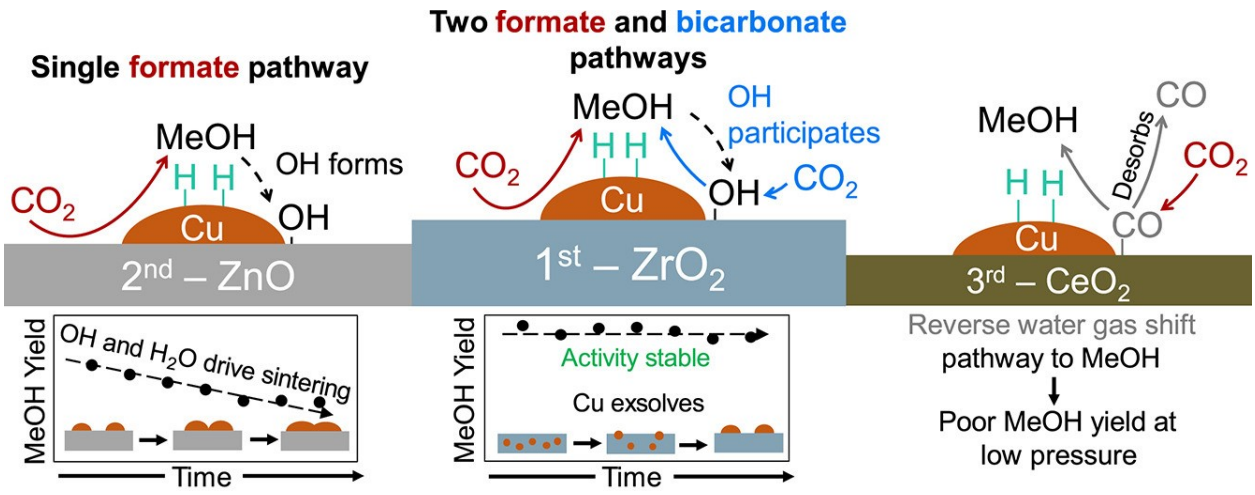


C4T: Mechanistic insights into the role of zinc oxide, zirconia and ceria supports in Cu-based catalysts for CO_2 hydrogenation to methanol

George Fulham, Xianyue Wu, Wen Liu, and Ewa Marek, *Chemical Engineering Journal*

DOI: 10.1016/j.cej.2023.147732

Abstract: Copper-based catalysts enable the hydrogenation of CO_2 to methanol (MeOH). Selective MeOH synthesis requires the interaction of copper with a metal oxide support to facilitate CO_2 adsorption and hydrogenation. Here, we systematically appraise the role of ZnO, ZrO_2 and CeO_2 in Cu-based catalysts for low-pressure (1 bar) MeOH synthesis. During temperature-programmed desorption (TPD) of CO_2, the bare ZnO, ZrO_2, and CeO_2 exhibited desorption events at both low (70–100 °C) and high (400–700 °C) temperatures, also observed when combining each support with copper. Investigations in a packed bed reactor showed suppressed CO by-production over Cu-ZrO_2, leading to a 1.5-fold improvement as compared to Cu-ZnO. Upon Cu-CeO_2, CO_2 was prone to undergo reduction to CO and desorb, resulting in a MeOH yield 9 times lower than over Cu-ZrO_2. Experiments aiming at intermittent operation with successive start-ups and shut-downs showed that the performance of Cu-ZrO_2 catalyst remained stable, whilst Cu-ZnO deteriorated monotonically, ascribed to sintering driven by OH and H_2O species. In situ infrared spectroscopy demonstrated that methanol synthesis over Cu-ZnO progresses via a single pathway with formate species, whilst parallel formate and bicarbonate pathways were demonstrated over Cu-ZrO_2. Unlike Cu-ZnO, the formation of bicarbonate over Cu-ZrO_2 allows surface OH species to participate in MeOH synthesis, which we link to the superior performance and stability of Cu-ZrO^2.

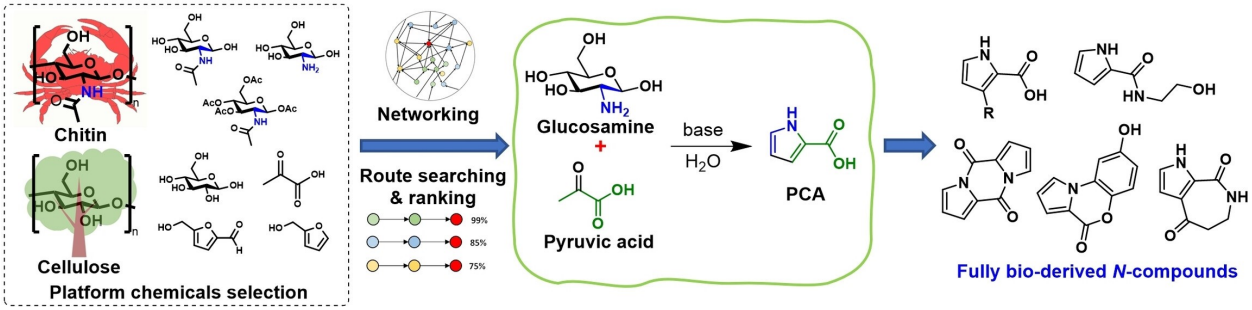


C4T: Synthesis of Pyrrole-2-Carboxylic Acid from Cellulose- and Chitin-Based Feedstocks Discovered by the Automated Route Search

Thuy Trang Pham, Zhen Guo, Bing Li, Alexei Lapkin, Ning Yan, *ChemSusChem*

DOI: 10.1002/cssc.202300538

Abstract: The shift towards sustainable feedstocks for platform chemicals requires new routes to access functional molecules that contain heteroatoms, but there are limited bio-derived feedstocks that lead to heteroatoms in platform chemicals. Combining renewable molecules of different origins could be a solution to optimize the use of atoms from renewable sources. However, the lack of retrosynthetic tools makes it challenging to examine the extensive reaction networks of various platform molecules focusing on multiple bio-based feedstocks. In this study, a protocol was developed to identify potential transformation pathways that allow for the use of feedstocks from different origins. By analyzing existing knowledge on chemical reactions in large databases, several promising synthetic routes were shortlisted, with the reaction of D-glucosamine and pyruvic acid being the most interesting to make pyrrole-2-carboxylic acid (PCA). The optimized synthetic conditions resulted in 50 % yield of PCA, with insights gained from temperature variant NMR studies. The use of substrates obtained from two different bio-feedstock bases, namely cellulose and chitin, allowed for the establishment of a PCA-based chemical space.



C4T: Investigation of barium iron oxides for CO_2 capture and chemical looping oxygen uncoupling

Syed Saqline, Haiming Wang, Qianwenhao Fan, Felix Donat, Christoph Müller, and Wen Liu,
Applications in Energy and Combustion Science

DOI: 10.1016/j.jaecs.2023.100238

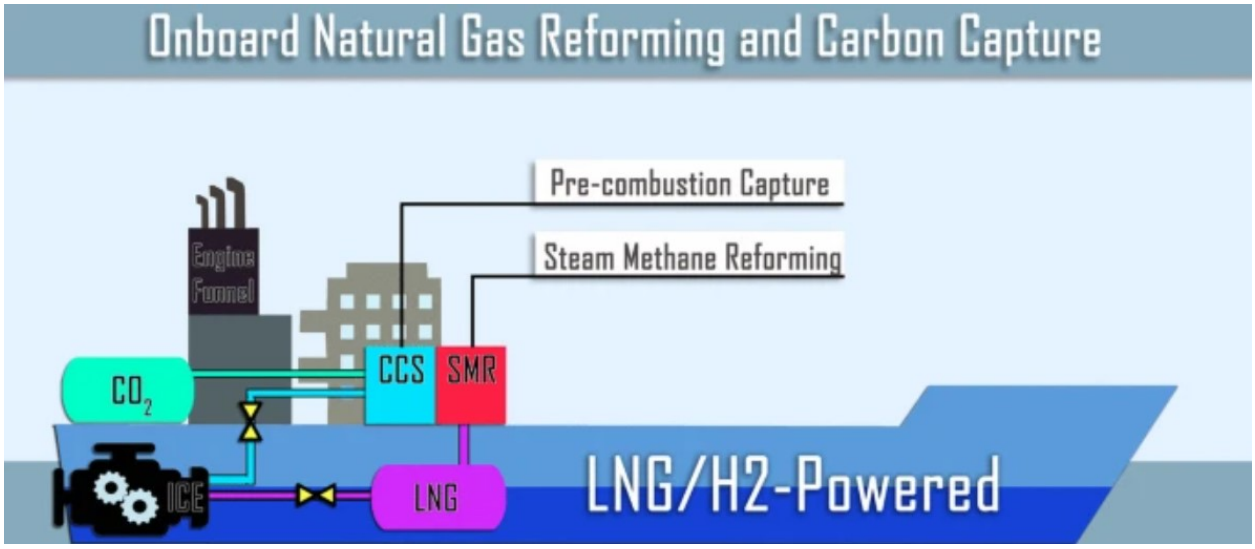
Abstract: The performance of two underexploited ternary oxides – $Ba_3Fe_2O_6$ and $Ba_5Fe_2O_8$ are investigated for carbon dioxide capture and chemical looping oxygen uncoupling. The ternary compound $Ba_3Fe_2O_6$ was found to have a structure characterised by space group $Pa3^{-}$. Experimental results have shown that both $Ba_3Fe_2O_6$ and $Ba_5Fe_2O_8$ are capable of cyclically capturing CO_2 at temperatures above 800 °C. $Ba_5Fe_2O_8$ demonstrated superior CO_2 capture performance compared to $Ba_3Fe_2O_6$, with consistent gravimetric CO_2 uptake capacities of 4.35 wt% and 13.39 wt% at 900 °C and 1000 °C, respectively, over 20 cycles. In comparison, $Ba_3Fe_2O_6$ demonstrated high initial CO_2 uptake capacities which deteriorated cyclically, with 20 cycle average capacities of 7.73 wt% and 11.99 wt% at 900 °C and 1000 °C, respectively. $Ba_3Fe_2O_6$ also exhibits excellent recyclability and satisfactory chemical looping oxygen uncoupling (CLOU) activity over temperature swing cycles between 550 °C and 950 °C. In contrast, the strong affinity with CO_2 makes $Ba_5Fe_2O_8$ unsuitable for application in chemical looping oxygen uncoupling or chemical looping air separation, especially in the presence of substantial partial pressures of CO_2.

C4T: A Thermodynamics Model for the Assessment and Optimisation of Onboard Natural Gas Reforming and Carbon Capture

Li Chin Law, Epaminondas Mastorakos, Mohd. Roslee Othman, and Antonis Trakakis, *Emission Control Science and Technology*

DOI: 10.1007/s40825-023-00234-z

Abstract: The paper examines pre-combustion carbon capture technology (PreCCS) for liquefied natural gas (LNG) propelled shipping from thermodynamics and energy efficiency perspectives. Various types of LNG reformers and CCS units are considered. The steam methane reformer (SMR) was found to be 20% more energy efficient than autothermal (ATR) and methane pyrolysis (MPR) reactors. Pressure swing adsorption (PSA) had a lower energy requirement than membrane separation (MEM), cryogenic separation (CS), and amine absorption (AA) in pre-combustion carbon capture, with PSA needing 0.18 kWh/kg CO_2. An integrated system combining SMR and PSA was proposed using waste heat recovery (WHR) from the engine, assuming similar efficiency for LNG and H_2 operation, and cooling and liquefying of the CO_2 by the LNG. The SMR-PSA system without WHR had an overall efficiency of 33.4% (defined as work at the propeller divided by the total LNG energy consumption). This was improved to 41.7% with WHR and gave a 65% CO_2 emission reduction. For a higher CO_2 reduction, CCS from the SMR heater could additionally be employed, giving a maximum CO_2 removal rate of 86.2% with 39% overall energy efficiency. By comparison, an amine-based post-engine CCS system without reforming could reach similar CO_2 removal rates but with 36.6% overall efficiency. The advantages and disadvantages and technology readiness level of PreCCS for onboard operation are discussed. This study offers evidence that pre-combustion CCS can be a serious contender for maritime propulsion decarbonization.



C4T: Potential and electric double-layer effect in electrocatalytic urea synthesis

Qian Wu, Chencheng Dai, Fanxu Meng, Yan Jiao, and Jason Zhichuan Xu, *Nature Communications*

DOI: 10.1038/s41467-024-45522-6

Abstract: Electrochemical synthesis is a promising way for sustainable urea production, yet the exact mechanism has not been fully revealed. Herein, we explore the mechanism of electrochemical coupling of nitrite and carbon dioxide on Cu surfaces towards urea synthesis on the basis of a constant-potential method combined with an implicit solvent model. The working electrode potential, which has normally overlooked, is found influential on both the reaction mechanism and activity. The further computational study on the reaction pathways reveals that *CO-NH and *NH-CO-NH as the key intermediates. In addition, through the analysis of turnover frequencies under various potentials, pressures, and temperatures within a microkinetic model, we demonstrate that the activity increases with temperature, and the Cu(100) shows the highest efficiency towards urea synthesis among all three Cu surfaces. The electric double-layer capacitance also plays a key role in urea synthesis. Based on these findings, we propose two essential strategies to promote the efficiency of urea synthesis on Cu electrodes: increasing Cu(100) surface ratio and elevating the reaction temperature.

C4T: Cross-domain flood risk assessment for smart cities using dynamic knowledge graphs

Markus Hofmeister, George Brownbridge, Michael Hillman, Sebastian Mosbach, Jethro Akroyd, Kok Foong Lee, and Markus Kraft, *Sustainable Cities and Society*

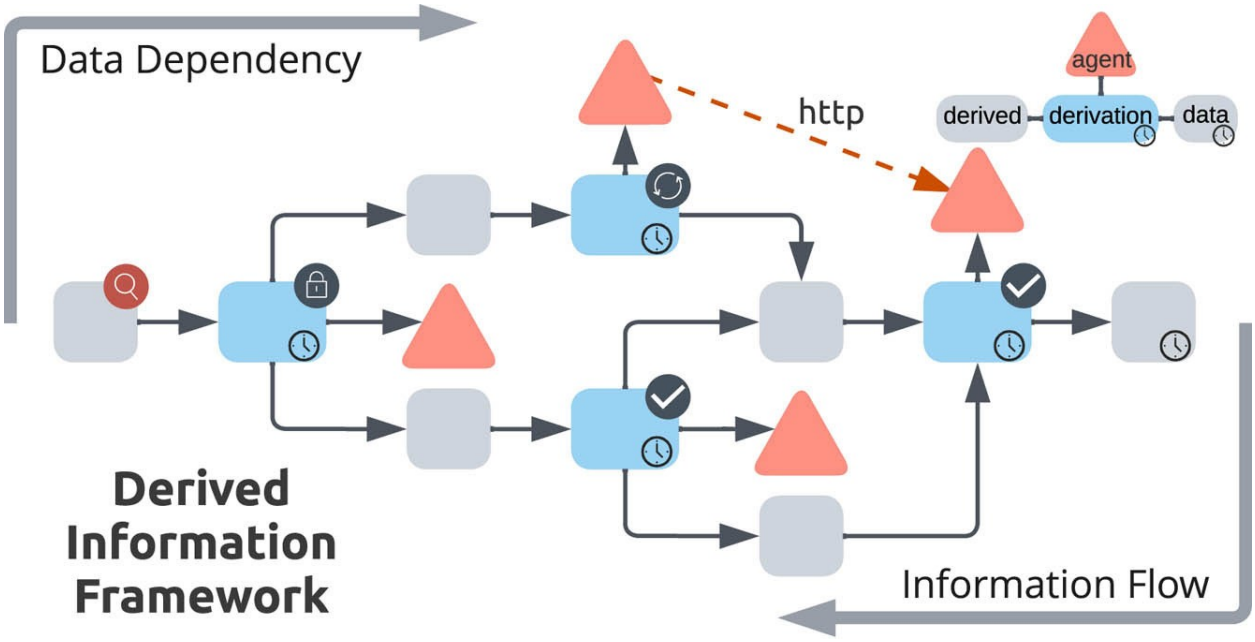
DOI: 10.1016/j.scs.2023.105113

Abstract: This paper investigates the usage of knowledge graphs to bridge the gap between current data silos in deriving a holistic perspective on the impact of flooding. It builds on the idea of connected digital twins based on the World Avatar dynamic knowledge graph to deploy an ecosystem of autonomous software agents to continuously ingest new real-world information and operate on it. Multiple publicly available yet isolated data sources, including geospatial building information and property sales data as well as real-time river levels, weather observations, and flood warnings, are connected to instantiate a semantically rich ecosystem of knowledge, data, and computational capabilities to provide cross-domain insights in projected flooding events and their potential impact on population and built infrastructure. The extensibility of the proposed approach is highlighted by further integrating power, water, and telecoms infrastructure as part of the very same system, in order to analyse flood-induced asset failures and their propagation across networks. The World Avatar promotes evidence-based decision making during several disaster management phases, supporting both tactical and strategic risk assessments, which supports the United Nations Sustainable Development Goal 11 to improve the assessment of vulnerability, exposure, and risk of communities imposed by flooding events.

C4T: A derived information framework for a dynamic knowledge graph and its application to smart cities

Jiaru Bai, Kok Foong Lee, Markus Hofmeister, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft,
Future Generation Computer Systems
DOI: 10.1016/j.future.2023.10.008

Abstract: In this work, we develop a derived information framework to semantically annotate how a piece of information can be obtained from others in a dynamic knowledge graph. We encode this using the notion of a "derivation" and capture its metadata with a lightweight ontology. We provide an agent template designed to monitor derivations and to standardise agents performing this and related operations. We implement both synchronous and asynchronous communication modes for agents interacting with the knowledge graph. When occurring in conjunction, directed acyclic graphs of derivations can arise, with changing data propagating through the knowledge graph by means of agents' actions. While the framework itself is domain-agnostic, we apply it in the context of smart cities as part of the World Avatar project and demonstrate that it is capable of handling sequential events across different timescales. Starting from source information, the framework automatically populates derived data and ensures they remain up to date upon access for a potential flood impact assessment use case.

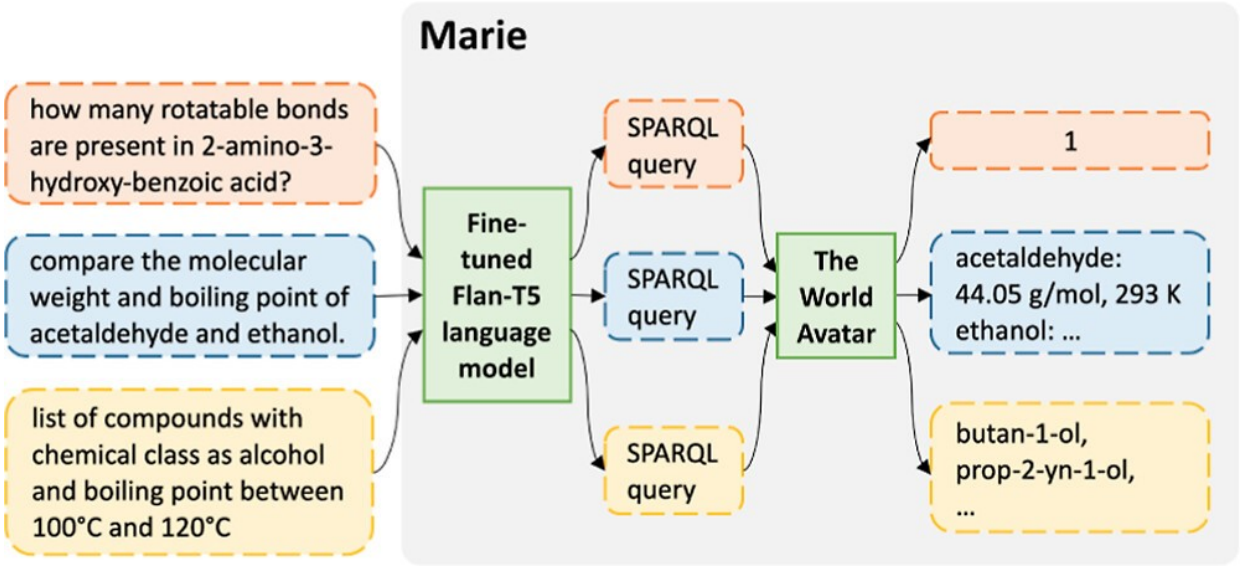


C4T: Leveraging Text-to-Text Pretrained Language Models for Question Answering in Chemistry

Dan Tran, Laura Pascazio, Jethro Akroyd, Sebastian Mosbach, and Markus Kraft, *ACS Omega*

DOI: 10.1021/acsomega.3c08842

Abstract: In this study, we present a question answering (QA) system for chemistry, named Marie, with the use of a text-to-text pretrained language model to attain accurate data retrieval. The underlying data store is "The World Avatar" (TWA), a general world model consisting of a knowledge graph that evolves over time. TWA includes information about chemical species such as their chemical and physical properties, applications, and chemical classifications. Building upon our previous work on KGQA for chemistry, this advanced version of Marie leverages a fine-tuned Flan-T5 model to seamlessly translate natural language questions into SPARQL queries with no separate components for entity and relation linking. The developed QA system demonstrates competence in providing accurate results for complex queries that involve many relation hops as well as showcasing the ability to balance correctness and speed for real-world usage. This new approach offers significant advantages over the prior implementation that relied on knowledge graph embedding. Specifically, the updated system boasts high accuracy and great flexibility in accommodating changes and evolution of the data stored in the knowledge graph without necessitating retraining. Our evaluation results underscore the efficacy of the improved system, highlighting its superior accuracy and the ability in answering complex questions compared to its predecessor.

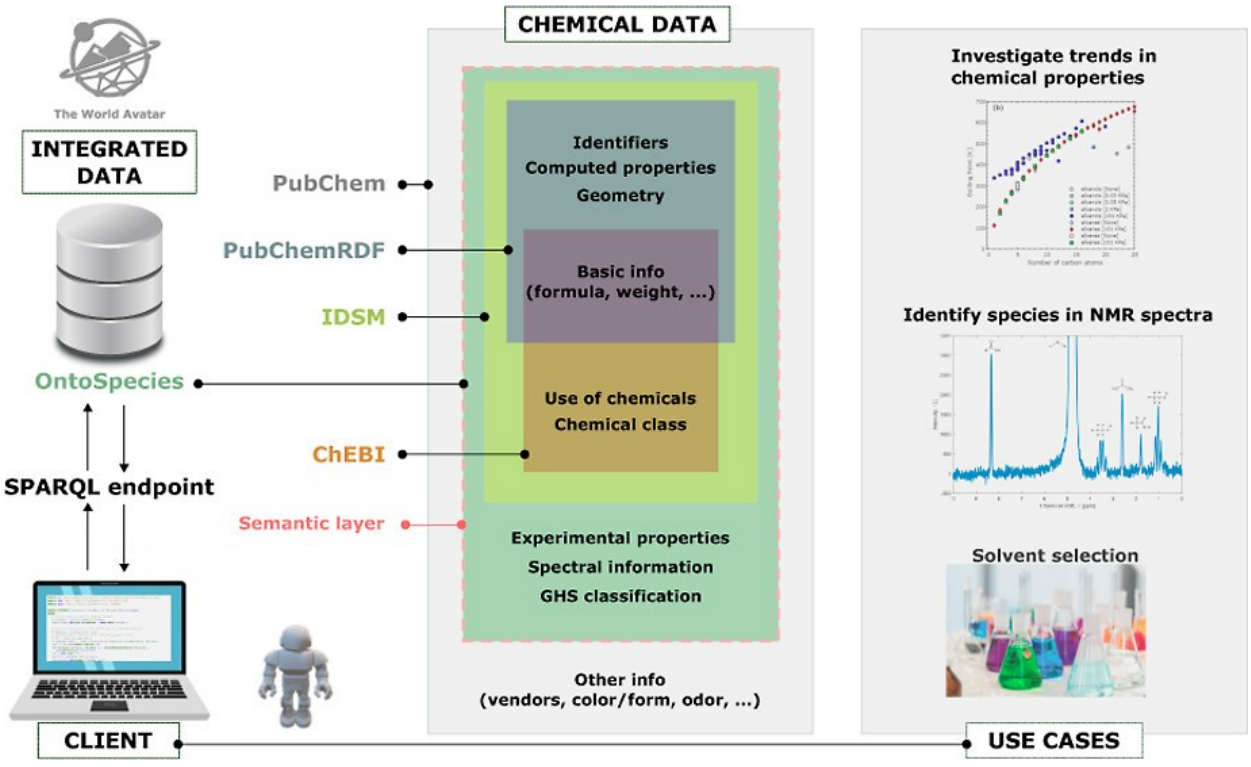


C4T: Chemical Species Ontology for Data Integration and Knowledge Discovery

Laura Pascazio, Simon Rihm, Ali Naseri, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *Journal of Chemical Information and Modeling*

DOI: 10.1021/acs.jcim.3c00820

Abstract: Web ontologies are important tools in modern scientific research because they provide a standardized way to represent and manage web-scale amounts of complex data. In chemistry, a semantic database for chemical species is indispensable for its ability to interrelate and infer relationships, enabling a more precise analysis and prediction of chemical behavior. This paper presents OntoSpecies, a web ontology designed to represent chemical species and their properties. The ontology serves as a core component of The World Avatar knowledge graph chemistry domain and includes a wide range of identifiers, chemical and physical properties, chemical classifications and applications, and spectral information associated with each species. The ontology includes provenance and attribution metadata, ensuring the reliability and traceability of data. Most of the information about chemical species are sourced from PubChem and ChEBI data on the respective compound Web pages using a software agent, making OntoSpecies a comprehensive semantic database of chemical species able to solve novel types of problems in the field. Access to this reliable source of chemical data is provided through a SPARQL end point. The paper presents example use cases to demonstrate the contribution of OntoSpecies in solving complex tasks that require integrated semantically searchable chemical data. The approach presented in this paper represents a significant advancement in the field of chemical data management, offering a powerful tool for representing, navigating, and analyzing chemical information to support scientific research.

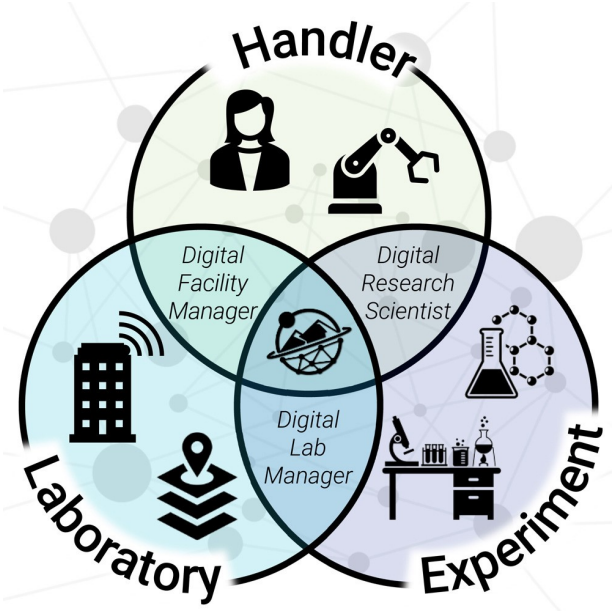


C4T: Transforming research laboratories with connected digital twins

Simon Rihm, Jiaru Bai, Aleksandar Kondinski, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *Nexus*

DOI: 10.1016/j.ynexs.2024.100004

Abstract: To substantially expedite scientific discovery, research laboratories need to be further automated. In this regard, the scientific community envisions an "artificial intelligence scientist" capable of planning, conducting, and assessing experiments based on higher-order goals and reasoning capabilities. We argue that a paradigm shift is necessary to bridge the gap between the current trajectory of lab automation and this vision. Adopting a systems perspective reveals several key challenges that must be addressed. We argue that achieving holistic lab automation requires a network of comprehensive distributed digital twins grounded in a universal knowledge model. Dynamic knowledge graphs are expected to play an important role, and we introduce a framework encompassing all aspects of experimental research, including infrastructure and peripheries. Our framework considers human-machine interactions from the outset to empower a goal-driven approach that brings automation to autonomy.



C4T: A dynamic knowledge graph approach to distributed self-driving laboratories

Jiaru Bai, Sebastian Mosbach, Connor J. Taylor, Dogancan Karan, Kok Foong Lee, Simon D. Rihm, Jethro Akroyd, Alexei A. Lapkin, and Markus Kraft, *ACS Omega*

DOI: 10.1038/s41467-023-44599-9

Abstract: The ability to integrate resources and share knowledge across organisations empowers scientists to expedite the scientific discovery process. This is especially crucial in addressing emerging global challenges that require global solutions. In this work, we develop an architecture for distributed self-driving laboratories within The World Avatar project, which seeks to create an all-encompassing digital twin based on a dynamic knowledge graph. We employ ontologies to capture data and material flows in design-make-test-analyse cycles, utilising autonomous agents as executable knowledge components to carry out the experimentation workflow. Data provenance is recorded to ensure its findability, accessibility, interoperability, and reusability. We demonstrate the practical application of our framework by linking two robots in Cambridge and Singapore for a collaborative closed-loop optimisation for a pharmaceutically-relevant aldol condensation reaction in real-time. The knowledge graph autonomously evolves toward the scientist's research goals, with the two robots effectively generating a Pareto front for cost-yield optimisation in three days.

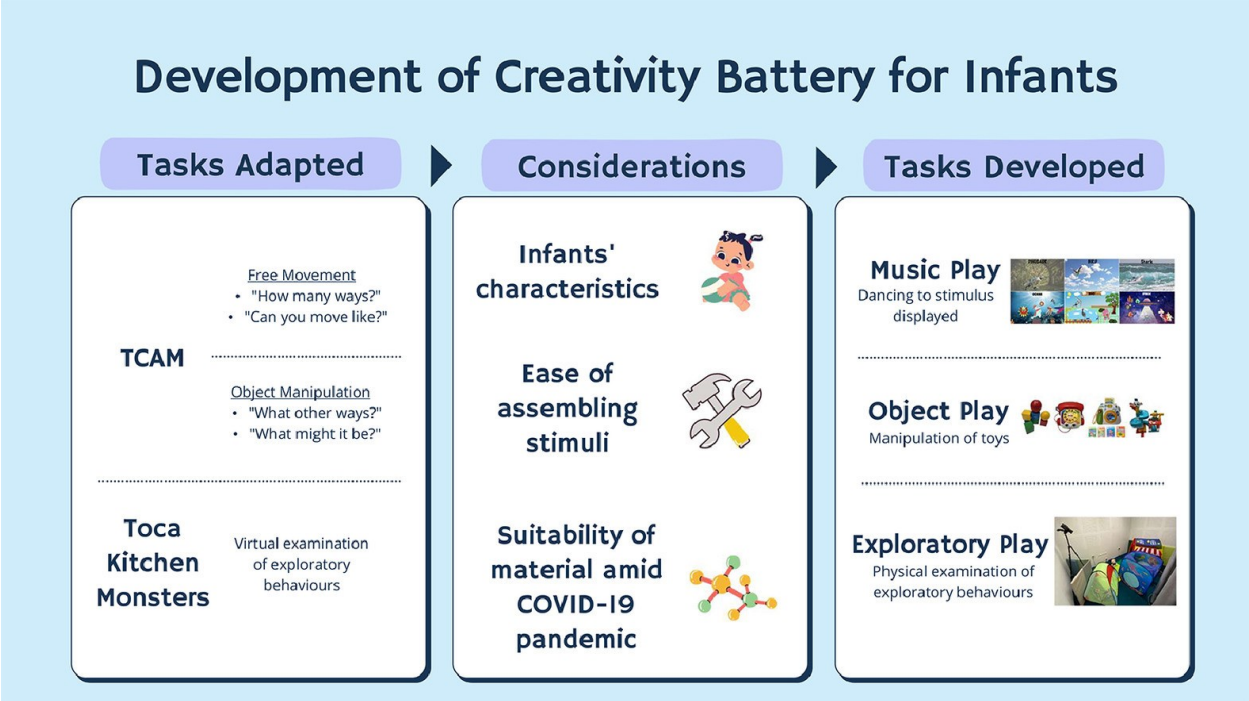
CLIC: Age-appropriate adaptation of creativity tasks for infants aged 12–24 months

Ling Zheng Teo and Victoria Leong, *MethodsX*

DOI: 10.1016/j.mex.2024.102655

Abstract: Creativity is an important skill that relates to innovation, problem-solving and artistic achievement. However, relatively little is known about the early development of creative potential in very young children, in part due to a paucity of tasks suitable for use during infancy. Current measures of creativity in early childhood include the Unusual Box Test, Torrance's Thinking Creatively in Action and Movement (TCAM) task and the Toca Kitchen Monsters task. These tasks are designed for children aged above 12, 36 and 18 months respectively, but very few measures of creativity can be used for infants aged below 2. Accordingly, here we report age-appropriate adaptations of TCAM and Toca Kitchen Monsters tasks for infants as young as 12 to 24 months. Considerations taken into account include (1) infants' cognitive capacities (i.e., attention span, language comprehension skills, motor skills, and approach to play), and (2) practicality of the stimuli, including suitability for use amid the COVID-19 pandemic. The modified creativity battery for infants includes three tasks: Music Play, Object Play and Exploratory Play tasks. The task protocols elaborated in this paper are intended to facilitate studies on the early development of creativity in infants aged between 12 and 24 months. Primary highlights include:

- Age-appropriate adaptation of creativity tasks for use with infants aged between 12 and 24 months.
- Consideration of infants' cognitive capacities and stimulus practicality.
- Innovative use of movement as expression of infants' creative behaviour.



PIPS: A machine learning-enabled process optimization of ultra-fast flow chemistry with multiple reaction metrics

Dogancan Karan, Guoying Chen, Nicholas Jose, Jiaru Bai, Paul McDaidd, and Alexei Lapkin, *Reaction Chemistry & Engineering*

DOI: 10.1039/D3RE00539A

Abstract: Discovering the optimum process parameters of ultra-fast reactions, such as lithium–halogen exchange reactions, is typically achieved by time and resource inefficient methods including one factor at a time optimization (OFAT) or classical factorial design of experiments (DoE). Herein, we demonstrate the development of a machine learning workflow coupled with a flow chemistry platform for the optimization of the reaction conditions of a lithium–halogen exchange reaction. Flow chemistry platform allowed us to precisely control the process parameters (temperature, residence time and stoichiometry) and enabled robust and reliable data collection to train a machine learning algorithm. A Bayesian multi-objective optimization algorithm TSEMO (Thompson sampling efficient multi-objective optimization) was used to optimize the process parameters and to build process knowledge for different optimization campaigns with different mixing intensifications (capillary reactor *vs.* microchip reactor). The algorithm successfully identified a set of optimal conditions corresponding the trade-off between yield and impurity in different optimization campaigns. Furthermore, the optimization results and Gaussian process (GP) surrogate models within TSEMO were further analyzed to infer the operating regime of the system for different mixing intensifications (mixing controlled *vs.* reaction-controlled regime). The machine learning workflow has proven to be robust and data efficient, revealing rich information about the reaction studied compared to single-objective, OFAT and DoE approaches.

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)

Dr Yu SHAO (Research Fellow, NTU) and **Asst Prof Paul LIU (PI, NTU)** have been working on the design and synthesis of a high entropy oxide (HEO) material, which serves as the catalyst and oxygen carrier for a chemical looping dry reforming of methane process (Figure 1.1a). The dry reforming of methane simultaneously converts two greenhouse gases (methane and carbon dioxide) into the syngas, a platform mixture for chemical industry. Meanwhile, integrating dry reforming of methane with chemical looping strategy effectively tackles operational difficulties such as thermodynamic limitations and side reactions. The high entropy oxide material exhibited outstanding catalytic activity and cyclic durability over 100 cycles of chemical looping reaction, in comparison to several medium entropy oxides and a benchmark nickel-iron oxide catalyst (Figure 1.1b, c). They have recently submitted a paper reporting the high entropy oxide catalyst and its application in carbon neutralisation.

In addition, Dr Shao and Asst Prof Liu have been working on several metal–organic framework (MOF)-based dual functional materials (DFMs) for an integrated carbon capture and conversion. In conventional carbon capture and storage processes (e.g., amine-media absorption), major energy consumption is associated with the desorption and compression. Hence, it is desirable to develop a material that is capable of CO_2 capture and *in situ* conversion. Two of developed DFM candidates displayed cyclic CO_2 uptakes of 9 and 13 wt%, respectively. Their current research endeavours focus on optimising the operating conditions for the conversion process.

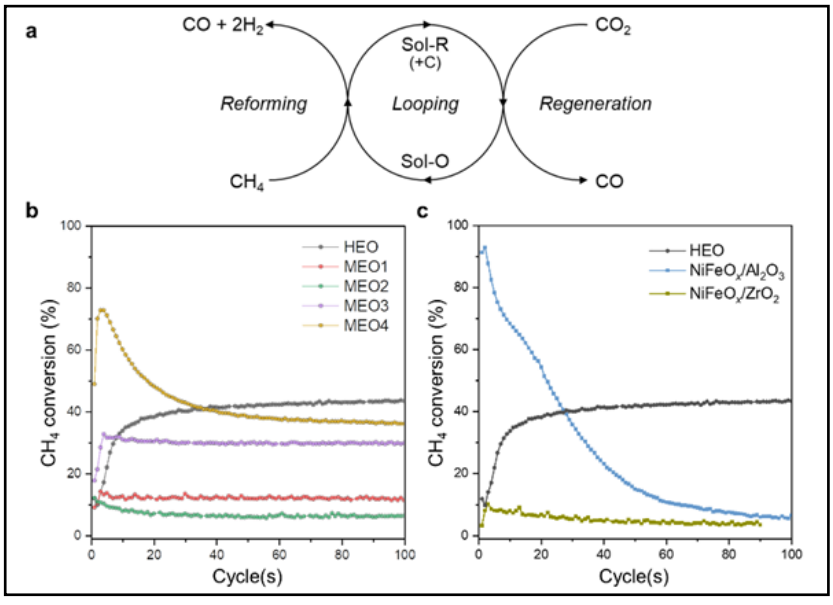


Figure 1.1: (a) Schematic illustration of the chemical looping dry reforming of methane process. (b, c) CH_4 conversion (%) per cycle for (b) HEO vs. MEOs and (c) HEO vs. NiFe-based catalysts.

Dr Yu SHAO

Dr Dara MOHAMED (Research Fellow, NTU) has been working on investigating the kinetics of aqueous phase CO_2 mineralisation of CaO in ammonium carbonate solution, a process involving three reaction steps, which are the (1) hydration of CaO to form $Ca(OH)_2$, (2) dissolution of $Ca(OH)_2$ in water and (3) precipitation of $CaCO_3$ from the aqueous Ca^{2+} and CO_3^{2-} species. Using the heat flow reaction calorimeter, the reaction progress can be observed in situ by measuring the heat flow generated during the reaction. The stirring speed, CaO batch size and pellet sizes were optimised and as shown in Figure 1.2a, a 300 rpm stirring speed and pellet size of 100-200 μm was sufficient to eliminate mass transfer limitations. The individual reaction steps were examined separately through calorimetry. It was found that the hydration step consisted of two stages for which the second stage is promoted as reaction temperatures increased, while the first peak is suppressed (Figure 1.2b). This phenomena affected the carbonation reaction at higher temperatures, as the second peak became more prominent, suggesting the kinetics do not favour higher temperatures. Through product analysis it was determined that the CO_2 mineralisation remained incomplete as unreacted $Ca(OH)_2$ was present in the product sample, suggesting the reaction proceeded via a shrinking core mechanism (Figure 1.2c). A technical disclosure for the know-how on using heat flow calorimetry for investigating the aqueous phase CO_2 mineralisation kinetics has been submitted. A manuscript summarising the findings in this study has also been prepared and recently been submitted for publication in *Chemical Engineering Science*.

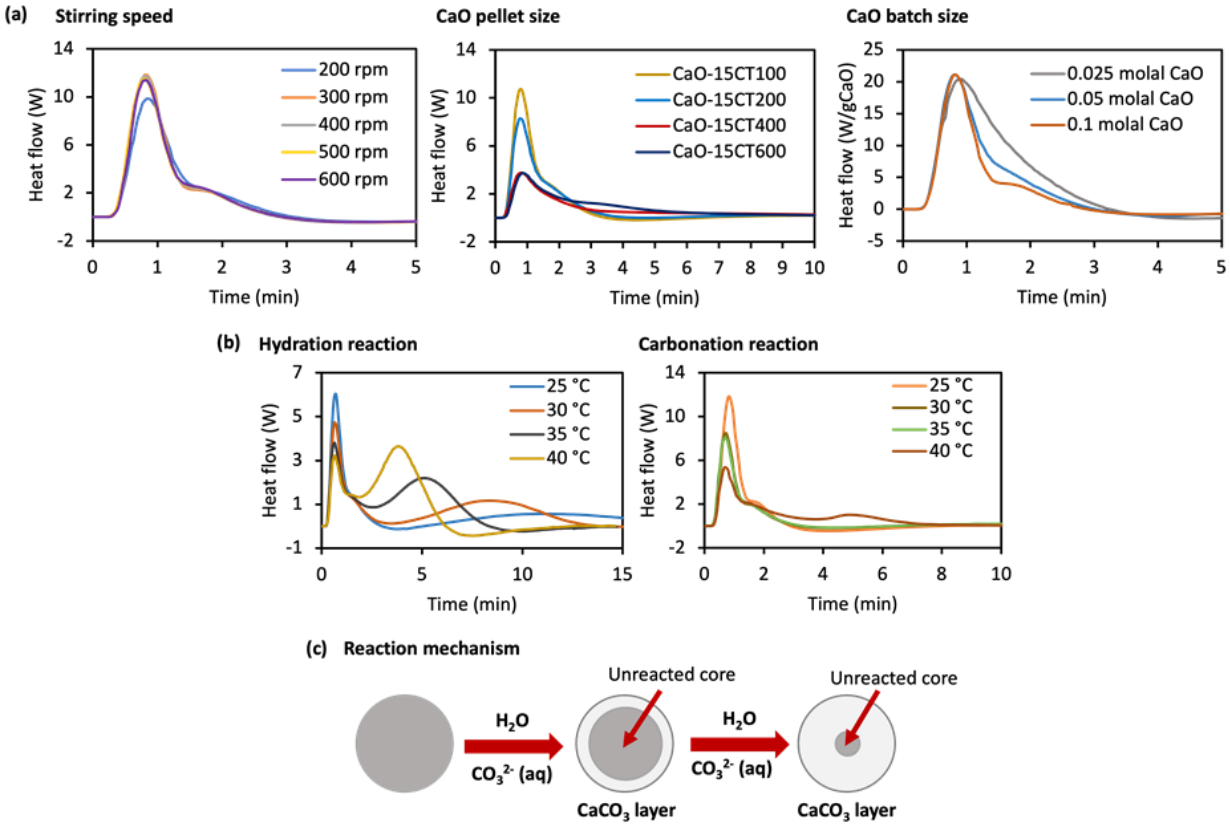


Figure 1.2: (a) Factors affecting rate measurements: stirring speed, CaO pellet sizes and CaO batch sizes. (b) Heat flow profiles of the hydration and carbonation reactions at different temperatures. (c) Shrinking core mechanism pathway for the aqueous carbonation of CaO in ammonium carbonate solution.

Dr Dara MOHAMED

Ms Xianyue WU (CARES Visitor, NTU) 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 working on a new research project to investigate the particle size and dispersion effects of Ni-based DFMs on their CO_2 capture and in-situ hydrogenation performance. She was adapting ethylene glycol (EG) and oleylamine method to synthesise Ni or NiO nanoparticles with different sizes. She discovered that the larger particle sizes of Ni would promote the CH_4 production during the hydrogenation step of the ICCU cycles, which is correlated to the conventional CO_2 hydrogenation performance. Recently, she was also investigating the H_2 partial pressure effect on reaction order of hydrogenation.

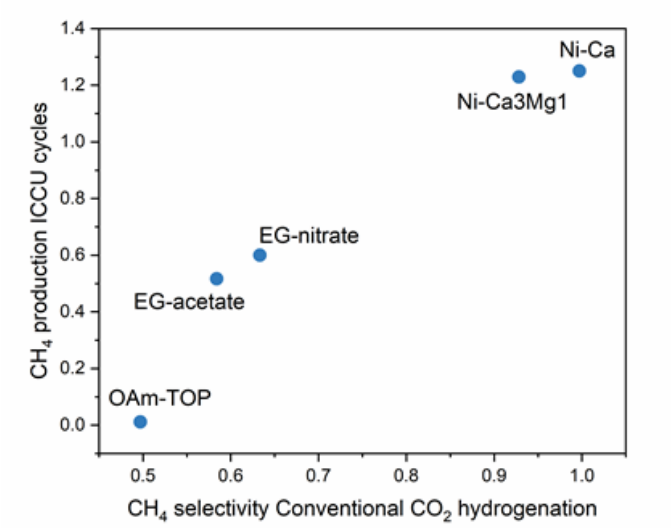


Figure 1.3: Correlation between CH_4 production during ICCU cycles and CH_4 selectivity during conventional CO_2 hydrogenation for different $Ni/CaCO_3$ based DFMs.

Ms Xianyue WU

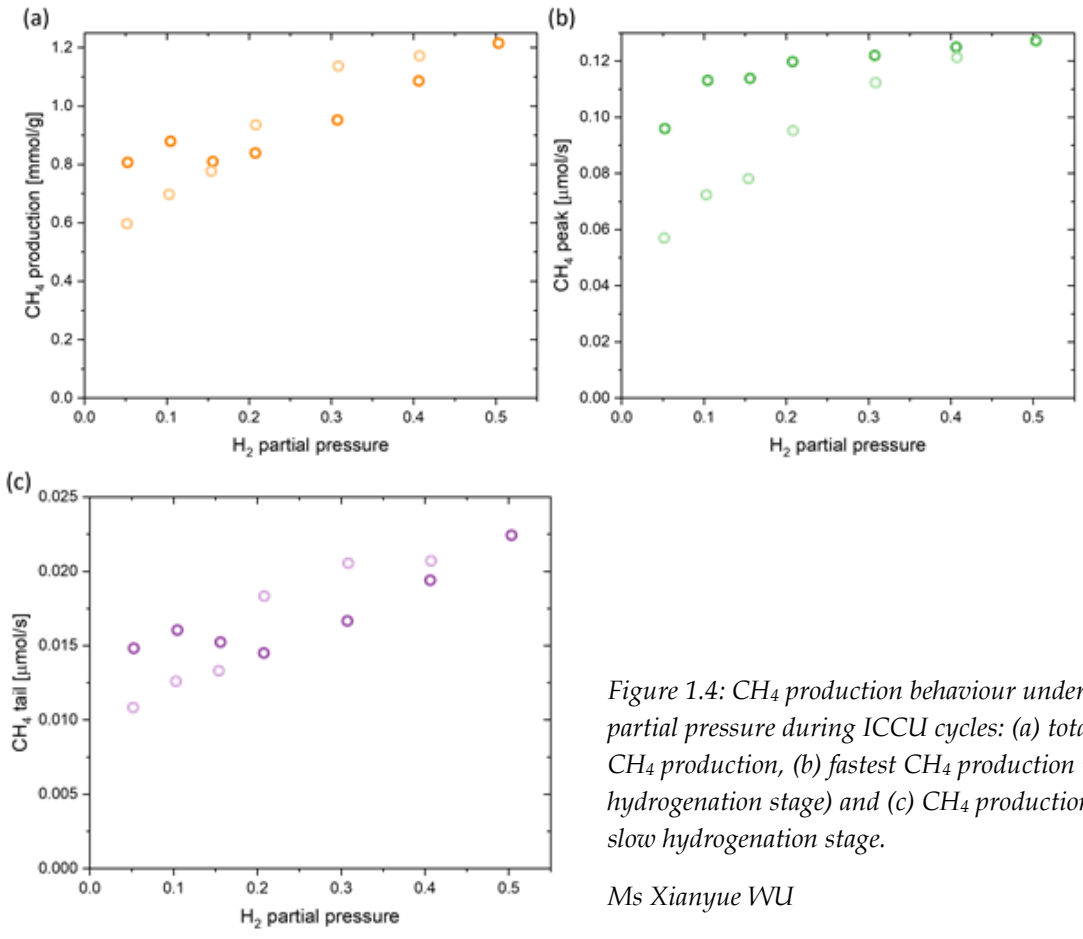


Figure 1.4: CH_4 production behaviour under different H_2 partial pressure during ICCU cycles: (a) total amount of CH_4 production, (b) fastest CH_4 production rate (fast hydrogenation stage) and (c) CH_4 production rate at the slow hydrogenation stage.

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 developed. This workflow was powered by physics-based regression models and neural networks, taken in conjunction. The workflow has been rigorously tested, and is now being implemented. The central hypothesis is that electronic metal/support interactions alter the properties of metal active sites. Such modified active sites exhibit reactivity, stability, and selectivity metrics that are different from metal sites considered separately.

Second, a set of scaling relationships (linear free energy relationships) to understand the selectivity of catalysts for the two-electron oxygen reduction were established. The selectivity trends inferred through these free energy relationships were compared with experiments. This work spans single- and dual-site catalysts comprising of earth abundant materials.

Third, a computational framework to simulate reactions under ultrasound irradiation was constructed. This framework predicts rates and selectivity of oxidation reactions, and determines the number density of free radical initiators generated during ultrasound irradiation.

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

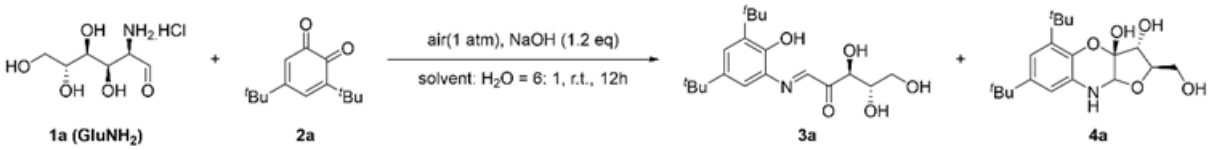
Prof Alexei LAPKIN (CAM)
Prof Ning YAN (NUS)

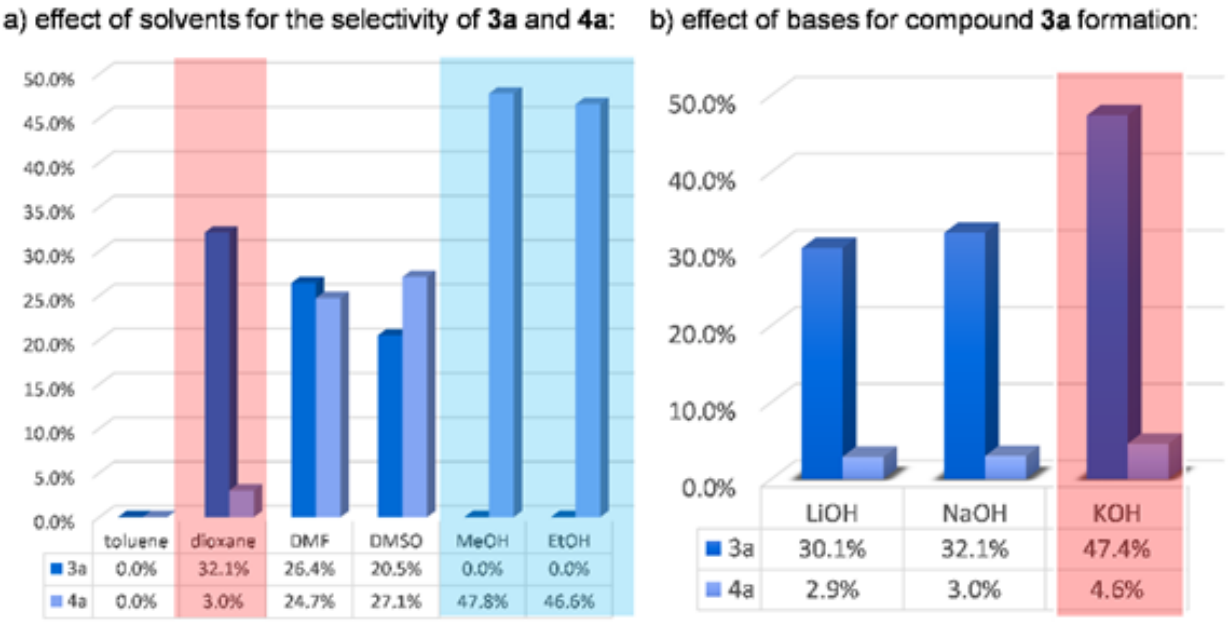
Guided by **Prof Alexei LAPKIN (PI, CAM)**, **Dr Zhen GUO (Senior Research Fellow, CARES)** has been collaborating with **Prof Ning YAN (PI, NUS)** on the discovery of low-carbon routes to functional molecules. Encouraged by the paper published on *ChemSusChem* in Oct 2023. The team started a new project on synthesis of fluorescent molecules from biowastes. Targeting Fluorescent brightener 185 as a case study, synthetic routes were extensively explored by taking advantage of our organic synthesis planner (CDI-CASP methodology). Synthetic routes using phenol, furfural and CO_2 as feedstocks were designed based on the searching results. Reactions were also proposed with the aid of searching of analogue reactions. **Dr Bing LI (Research Fellow, NUS)** was working on the experimental verifications in Prof Yan's lab.

In addition, Dr Guo also refurbished the database of CASP system by inserting new data. New data was generated and compiled in tables to facilitate searching in order to cope with the large dataset. Dr Guo will continue working with Prof Yan's team and conduct new searches based on feedback and develop algorithms to speed up searching of synthetic routes.

Dr Li focused on the synthesis of fluorescent whitening agents derived from glucosamine via biomimetic oxidation. Significant progress was made in optimising reaction conditions to achieve high selectivity of compound 3a, a crucial intermediate in the synthesis of the target fluorescent whitening agent. He used compound 2a as the substrate for condition screening in initial experimentation. Notably, the impact of solvent on selectivity was investigated, the results illustrated in Figure 1.5a. Aprotic solvents, such as dioxane, exhibited a favourability towards the formation of compound 3a, while protic solvents, including methanol and ethanol, promoted the generation of compound 4a (by-product). Further investigations into reaction efficiency unveiled the influence of the cation of the base, as demonstrated in Figure 1.5b. When potassium hydroxide was utilised as the base, a notable 47.4% yield of compound 3a was achieved. Dr Li also explored the

quantity varying of compound 2a to enhance selectivity, depicted in Figure 1.5c. Specifically, the utilisation of 3.0 equivalents of quinone resulted in an impressive 78.4% selectivity of compound 3a, thereby providing a robust foundation for subsequent synthesis steps toward fluorescent whitening agents.





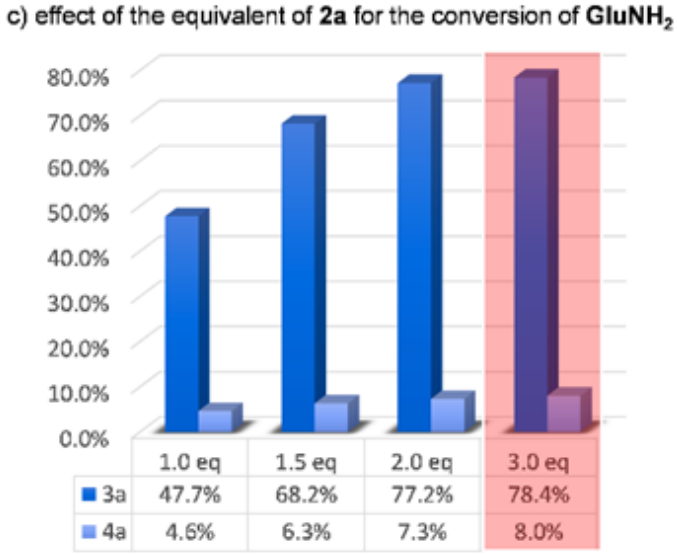


Figure 1.5: Optimisation of intermediates 3a synthesis for fluorescent whitening agents

Dr Bing LI

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) has been focused on identifying sustainable routes from biowaste to value-added chemicals using networks and knowledge graphs. He has further extended the knowledge graph to cover ~90 types of biomass (from Oil Palm Empty Fruit Bunch (EFB) to corn stover), ~40 pretreatment processes (from organic solvent processes, to ionic liquid processes), and ~120 feedstocks (from lignin to chitin). He has also extended the knowledge graph to include a reaction network containing ~300,000 chemical reactions from biowaste feedstocks to value-added chemicals, mined and cleaned from the Reaxys database.

Having obtained and represented the data, the next step is to evaluate the sustainability of various pathways in the graph for extraction of feedstocks from biowaste samples. To this end, various metrics were explored ranging from carbon emissions, cost, energy demand and energy efficiency, to exergy demand (taking into account entropy as well) and exergy efficiency. As exergy is an underexplored yet relevant metric, it was further expanded on. An exergy databank of more than 300 pure chemical species was assembled from literature as well as correlations for exergy calculations of more complex mixtures. This has been integrated with open-source python-based process simulators like Biosteam which represent and simulate process networks obtained from the existing knowledge graph.

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 been initiated. The aim is to leverage LLMs for knowledge retrieval and extraction (relevant entities and relationships for the knowledge graph) over a large literature corpus, further scaling the knowledge graph in an automated manner.

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 investigated voltage-controlled nanofiltration and how it provides a promising avenue for precise and on-demand molecular separation. This technique has been rarely reported in organic solvent nanofiltration (OSN) due to the concerns about the lower dielectric constant of organic solvents. The group fabricated conductive and robust conjugated microporous polymer (CMP) membranes by electropolymerisation. The resulting membranes present good conductivity and stability. The membranes were then evaluated in the OSN process in conjunction with electric field (Figure 2.1). Leveraging the significant electrostatic repulsion effect induced by applied voltage, the group observe a remarkable voltage gating behaviour on the permeation of charged molecules, thereby enhancing their rejection in situ. Different solvents were also used, showing a direct dependence of rejection enhancement by voltage on the dielectric constant of the solvents.

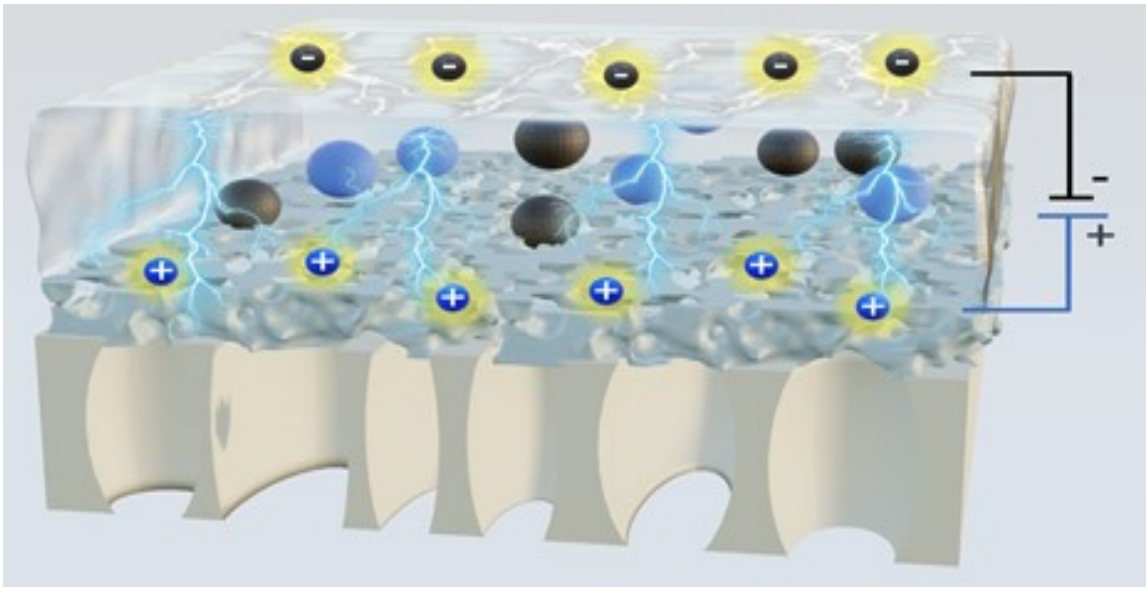


Figure 2.1: An illustration of the voltage-controlled OSN process.

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 the prospect of generating hydrogen through water electrolysis. The process 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 electrolysers faces challenges in achieving industrial-scale current densities as well as in addressing crossover issues. Here, we present an innovative acid-alkali asymmetric cell design to suppress the crossover of liquid products and facilitate GOR. Such device also demonstrates the capability of impeding C-C bond cleavage to promote high-value C3 products generation and reduce carbon emission. 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}.

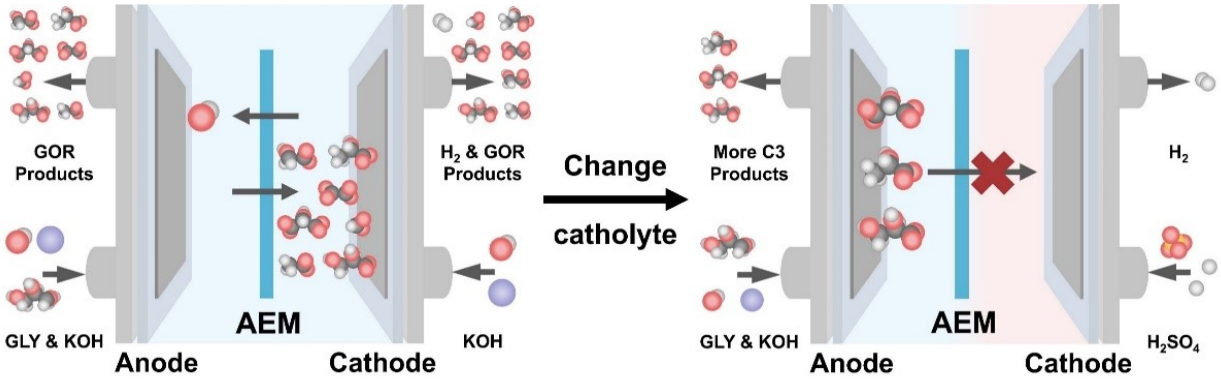


Figure 2.2: Graphical schematics of the AEM-based alkali-alkali and acid-alkali MEA devices. The acid-alkali MEA cell show capability of suppressing the product anion crossover and C-C bond cleavage.

Dr Chencheng DAI

ALTERNATIVE ENERGY

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

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

Decarbonising the energy sector through the transition towards low- or zero-carbon fuels is essential to meet Singapore's target of achieving net-zero emissions by 2050. One such transition is the introduction of new hydrogen-rich town gas to the residential and commercial cooking sectors. However, the combustion properties of the new hydrogen-rich town gas in cook stoves have not been studied in Singapore. Therefore, the project aims to identify the combustion properties associated with using the new hydrogen-rich town gas. The primary focuses are on developing standardised methods for hydrogen combustion diagnostics and studying the emissions from different gas compositions and stove types.

During this reporting period, the team conducted a literature review on prevailing test projects and established hydrogen safety standards. The literature review revealed that in the last 10 years, pilot projects have been carried out worldwide involving the mixing of hydrogen with natural gas. The proportion of hydrogen in natural gas typically ranges from 5% to 30%, with 20% being the highest blending ratio currently used by most countries.

The introduction of hydrogen into the urban gas pipeline network also presents several considerations. Key among these is ensuring compatibility with existing infrastructure, maintaining integrity to prevent leaks or failures, and mitigating any additional risks associated with hydrogen embrittlement. For terminal users, the shift to hydrogen-rich gas as a fuel source impacts terminal burners, raising questions about fuel interchangeability and safety. This includes evaluating the efficiency and emissions of burners when operated with hydrogen-rich gas and ensuring that safety standards are met or exceeded to handle hydrogen's wider flammability range and higher burning velocity.

Following the literature review, the team designed a measurement workflow tailored for emission measurement of high hydrogen content flame in the laboratory. A risk assessment of the design was also conducted to ensure a safe workflow in the laboratory. According to the workflow, the town gas cylinder will first be stored in the gas cylinder room before setting up the gas line leading to the fume hood, where a leak check will be performed. A check will also be performed to ensure that the fuel tubes, cook stoves, and sampling apparatus are properly connected. Once all the gases are confirmed to be flowing correctly, the flame will be ignited with a butane torch. The flame is allowed to stabilise for at least 10 minutes, during which the flame and gas flow rates will be carefully monitored. Once the flame has stabilised, an online gas analyser will be initiated to measure emissions. The exhaust gas from the flame will also be collected into a denuder for offline measurement. After the completion of the experiment, the flame will be extinguished, and all the gases, sampling equipment and power sources will be turned off.

The team also explored the combustion characteristics of hydrogen-methane mixtures by employing chemical kinetics models, specifically GRI-Mech 3.0. Figure 3.1 shows the four key characteristics of hydrogen-natural gas combustion (flame speed, flame temperature, NO_x emissions, and hydroxyl (OH) mole fraction) plotted against varying mixing ratios of hydrogen to natural gas.

These graphs not only serve as a foundation for understanding the dynamics of hydrogen-natural gas combustion, but also serve as the benchmark for the experiments in the next stage of the project.

The flame speed graph shows that the flame speed is directly proportional to the hydrogen content in the mixture. This phenomenon can be attributed to hydrogen's low ignition energy and high diffusivity, which enhance the flame propagation rate. The results indicate that even modest incorporations of hydrogen into natural gas can substantially elevate combustion efficiency. The flame temperature graph shows a gradual ascent in temperature with an increase in the hydrogen content. This increment could potentially translate into higher thermal efficiencies for combustion systems. The NO_x emissions graph shows that the level of emissions increases as the hydrogen content increases, primarily due to the elevated flame temperatures associated with hydrogen combustion, which favors the formation of nitrogen oxides. Lastly, the OH mole fraction graph provides insights into the chemical kinetics of the combustion process. The rising trend in OH mole fraction with increased hydrogen content suggests a more reactive combustion environment. OH radicals play a pivotal role in combustion chemistry, facilitating faster reaction rates and contributing to the overall efficiency of the combustion process.

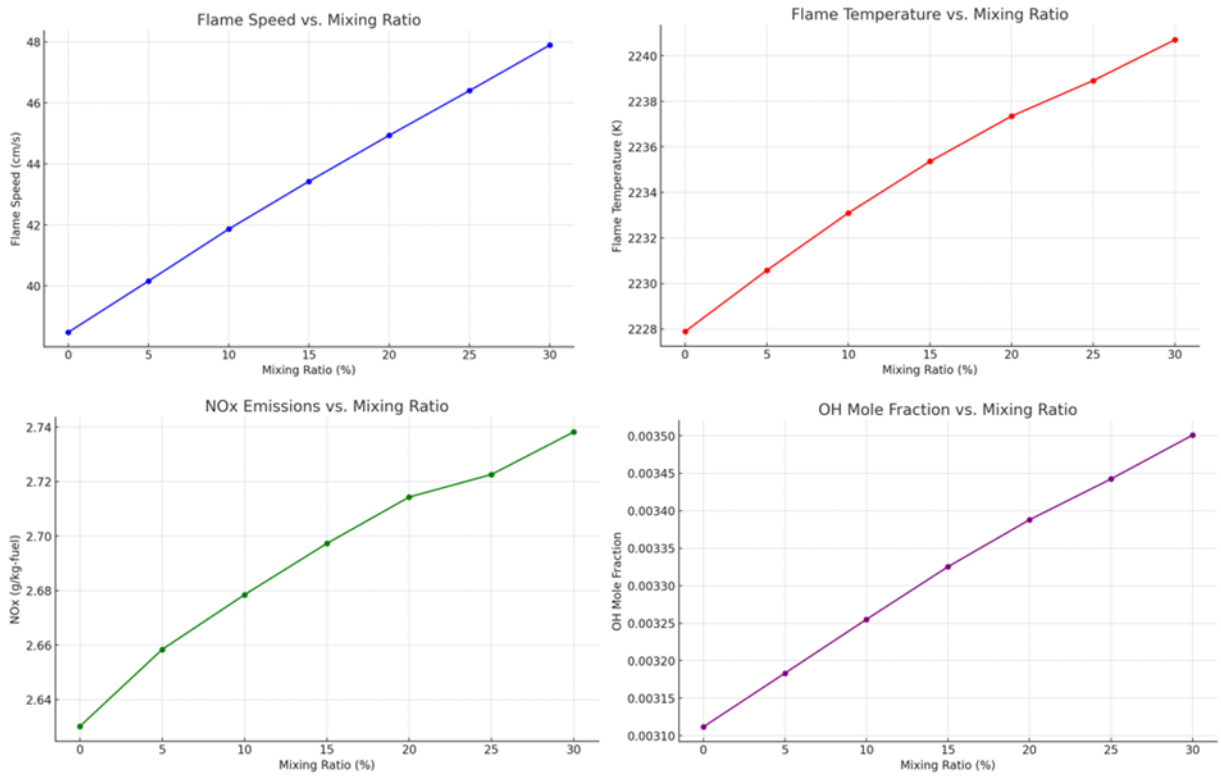


Figure 3.1: Flame and emission properties against varying hydrogen-natural gas ratio.

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

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

The 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. H18-DBT undergoes dehydrogenation under a palladium or platinum-based catalyst to release nine moles of H_2 (Figure 3.2). Numerous existing studies have developed novel catalysts for the dehydrogenation of H18-DBT.

During this reporting period, the team created platinum (Pt)/ titanium dioxide (TiO_2) catalysts using flame synthesised TiO_2 nanoparticles as a support and investigated its performance. Flame-synthesised TiO_2 nanoparticles have high oxygen vacancies as they are synthesised in oxygen-lean conditions. This enhances their catalytic performance due to enhanced electron transport and improved surface chemical properties of the catalysts. Therefore, Pt/TiO_2 catalysts using flame-synthesised TiO_2 could enhance the dehydrogenation rates of H18-DBT.

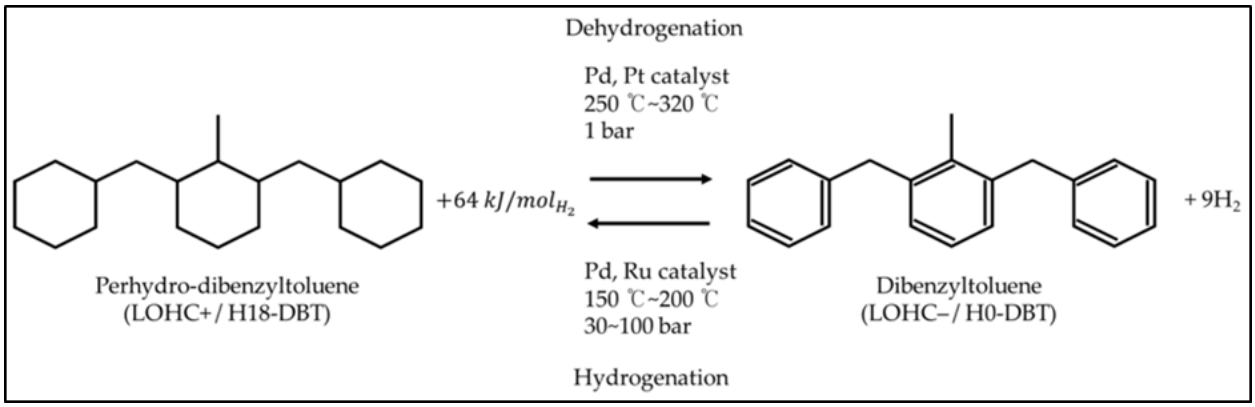


Figure 3.2: Dehydrogenation and hydrogenation of H18-DBT.

A schematic of the flame synthesis system designed by the team is shown in Figure 3.3. A premixed gas comprising of 20 slpm of compressed dry air (CDA) and 1.6 slpm of ethylene (C_2H_4) was used and ignited. To stabilise the flame, 20 slpm of nitrogen (N_2) gas was injected to maintain a stable ignited gas flow. After the flame stabilised for 10 minutes, the titanium precursor, titanium isopropoxide (TTIP), was injected using a syringe at a rate of 0.5 ml/min. Oxygen-lean TiO_2 was deposited onto a rotating stainless-steel disk, which is cooled by a flow of 50 lpm of CDA. To ensure the oxygen-lean state of TiO_2, a particle collection system is employed to collect the deposited TiO_2 particles before undergoing additional rounds of heating under the flame. The particle collection system comprises a heat-resistant scraper that continuously scrapes the surface of the rotating disk, along with a small stream of CDA (3.5 slpm) to remove TiO_2 particles into a collection bowl.

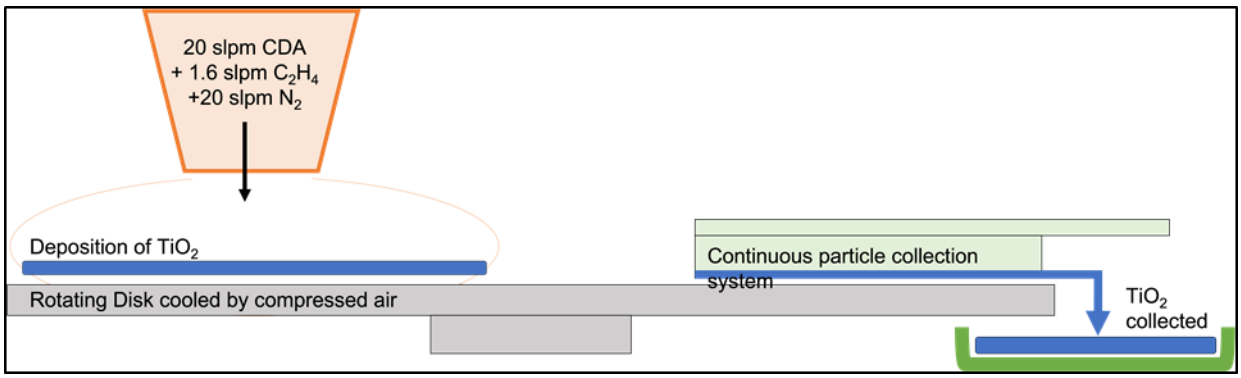


Figure 3.3: Schematic of the flame synthesis system.

Pt/TiO_2 catalysts were prepared using wet impregnation with aqueous solutions of a Pt precursor ($Pt(NH_3)_4(NO_3)_2$) and TiO_2 supports. The metal precursor was dissolved in 10 ml of deionised water and mixed for 3 hours. The solution was then dried in a 110°C oven overnight and calcined in a muffle furnace at 400°C for 4 hours, with a ramp rate of 5°C/min. Subsequently, the catalysts were reduced under H_2 for 2 hours at 400°C, with a flow rate of 15 ml/min.

All dehydrogenation experiments were conducted in a 250 ml three-neck glass flask at 310°C for 90 minutes, with a substrate-to-Pt ratio of 3,000. A gas flow inlet and outlet were connected to the left and right necks of the flask, respectively, with a thermocouple submerged into the central neck. A heating mantle was used to ensure good contact between the flask and the heating source. A glass stirrer bar was added to facilitate reactor stirring. After purging the setup with H_2, the reaction was initiated and carried out for 90 minutes, with the dehydrogenation rate monitored by a mass flow meter. After 90 minutes, the reactor was cooled, and a sample of DBT was retrieved for dehydrogenation rate analysis using Gas Chromatography-Mass Spectrometry (GCMS).

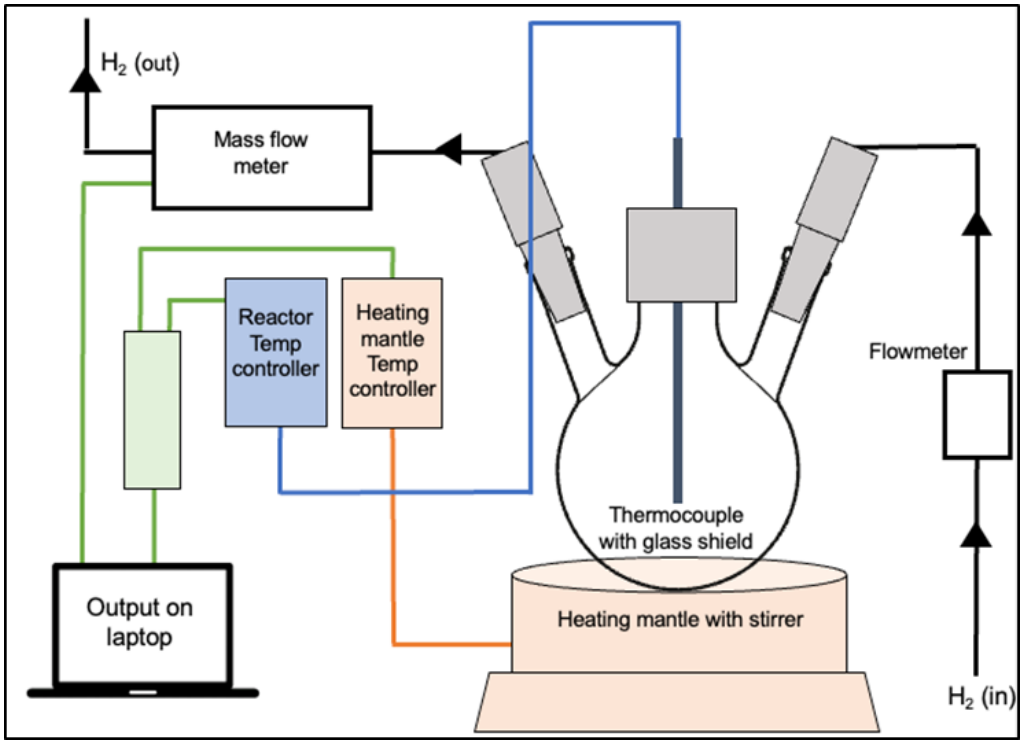


Figure 3.4: Schematic of the dehydrogenation setup.

Figure 3.5 illustrates the degree of dehydrogenation (DoD) results for flame-synthesised Pt/TiO_2 catalysts against commercial Pt/TiO_2 catalysts for different Pt loadings. It is observed that at most Pt loadings, the flame-synthesised Pt/TiO_2 catalysts exhibited comparable or even higher catalytic activity compared to the commercial Pt/TiO_2 catalysts. For the Pt loading of 0.2 wt%, the flame-synthesised catalyst displayed a slightly lower activity of 54.6%, compared to the activity of 60.4% for the commercial catalyst. However, as the Pt loading increases to 3.0 wt%, the flame-synthesised catalysts exhibited significantly higher catalytic activity compared to the commercial catalysts. The loading of 0.4 wt% and 0.3 wt% was shown to be the optimal Pt loading for commercial catalysts and flame-synthesised catalysts respectively. The results suggest that, even though flame synthesised TiO_2 support has higher oxygen vacancies, it may not necessarily exhibit better performance. Additionally, suboptimal Pt loading, or poor dispersion of Pt particles can limit the availability of active sites for the dehydrogenation reaction, thereby affecting the overall performance of the catalyst.

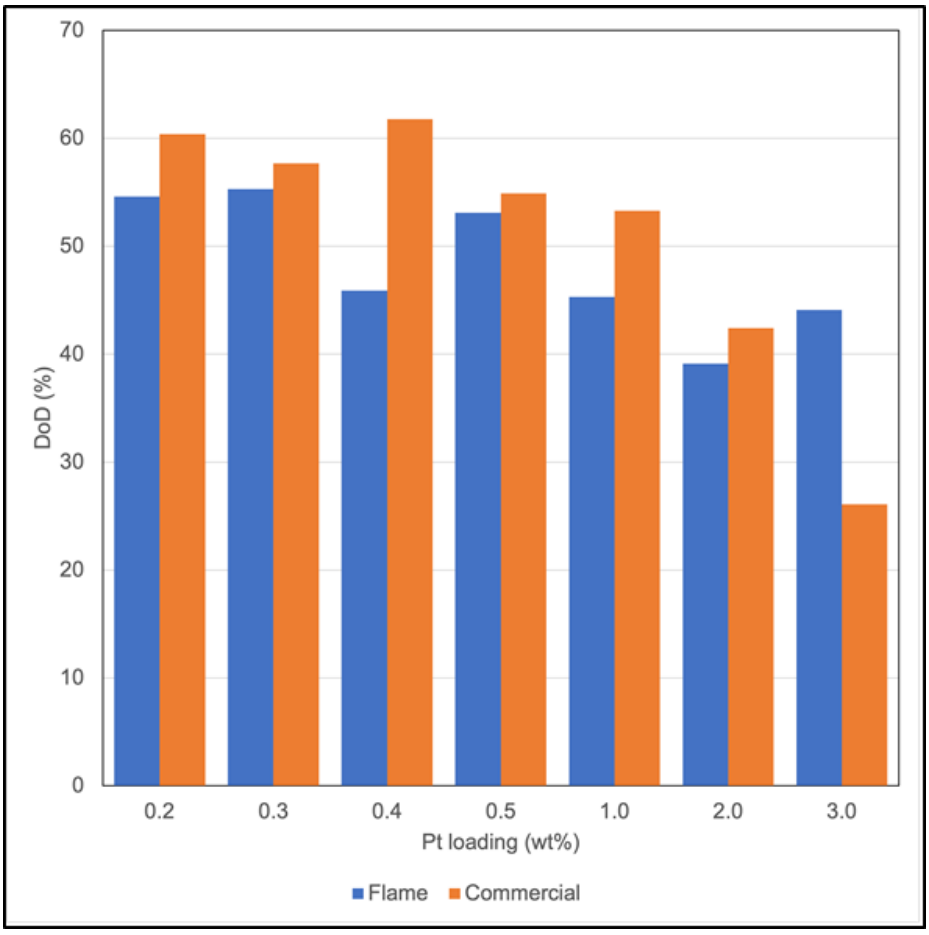


Figure 3.5: The degree of dehydrogenation (DoD) performance of perhydro-dibenzyltoluene (H18-DBT) over flame -synthesised Pt/TiO_2 catalysts and commercial Pt/TiO_2 catalysts.

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 worked on creating new GDE designs. High-current-density-induced failures in electrochemical CO_2 reduction flow cells are concluded to result from challenges in mass transport, electrolyte conductivity, and electrode stability. Flooding is a critical problem that arises as conventional carbon papers commonly used in GDE designs tend to lose their hydrophobicity over time at high current densities during the CO_2 reduction reaction (CO2RR). Upon losing hydrophobicity, the liquid electrolyte blocks the gas diffusion pathways for CO_2, reducing the availability of CO_2 at the electrocatalytic sites and facilitating the promotion of the hydrogen evolution reaction (HER). Notably, the hydrophobicity of the catalyst can also significantly accelerate such unwanted side reactions in the HER pathway. Adjusting both substrate and catalyst surface hydrophobicity has been proven effective in suppressing these issues.

To tackle substrate-related challenges, the team opted for a solution that substitutes carbon paper with a polytetrafluoroethylene (PTFE) membrane, renowned for its enduring and high hydrophobic characteristics, and addition of Copper (Cu) to form an integrated PTFE membrane – Cu GDE. In this integrated design, the PTFE membrane is employed as the gas diffusion layer and the Cu foam serves as a catalyst layer directly on top of the PTFE membrane. Using the Cu foam offers advantages, including exceptional conductivity and the potential for high-temperature post -treatment of electrodes. The team also devised a method to seamlessly integrate these disparate components, resulting in a unified GDE system.

The copper oxide (CuO) in the GDE was synthesised by galvanostatic anodic oxidation of the Cu mesh. Copper hydroxide ($Cu(OH)_2$) was primarily generated on the Cu surface during anodic oxidation, with the $Cu(OH)_2$ being spontaneously converted to CuO at the appropriate current density. The team discovered that an appropriate current density resulted in the best catalyst performance. Excessive current can lead to rapid Cu $(OH)_2$ production, resulting in complete coverage of the blue $Cu(OH)_2$ on the surface. Conversely, insufficient current generated only a thin oxide layer rather than nanosheet arrays.

The team prepared different experimental samples with varying anodisation times of 1, 3, 8, and 12 hours, resulting in different morphologies and crystalline phases of CuO. An 8-hour anodisation led to the formation of ultrathin CuO nanosheets with numerous exposed catalytically active sites during electrocatalysis. Shorter anodisation times resulted in incomplete growth of the CuO nanosheets on the surface of the electrode. Furthermore, the team conducted a Scanning Electron Microscopy (SEM) analysis on the experimental samples and concluded that increasing the current density during the anodisation process changes the morphology from nanosheets to nano-needles. However, it was observed that the nano-needles did not exhibit good performance for electrochemical CO_2 reduction.

Additionally, the team employed an X-Ray Diffraction (XRD) pattern analysis on the experimental samples to elucidate the crystal structures of the various electrodes. The Cu mesh exhibited three distinctive diffraction peaks at 42.5°, 49.3°, and 73°, corresponding to the (111), (200), and (220) planes of Cu, respectively. Following anodisation for a duration of 3 hours, two additional diffraction peaks appeared at 35.4° and 38.6°. The minor diffraction peak at 35.4° was attributed to the (-111) plane of CuO, while the prominent peak at 38.6° was assigned to the (111) plane of CuO. Subsequently, prolonging the anodisation time to 8 hours resulted in the sharpening of the

peaks. The XRD analysis of CuO nanosheets affirmed the successful synthesis of CuO without any discernible impurities, such as $Cu(OH)_2$ and Cu_2O.

Moreover, augmenting the current density during the anodisation process of the Cu mesh led to the emergence of two new peaks at 16.6° and 24°. These peaks were indicative of the formation of $Cu(OH)_2$ at higher current densities. Additionally, it became evident that the intensity of the peaks attributed to CuO was diminishing with the increase in current density.

The team also evaluated the application potential of as-prepared GDEs for industrial CO_2RR by measuring their catalytic performance in a flow cell. A commercial flow cell electrolyser was used for the electrochemical CO_2RR test. The GDEs were placed between the gas chamber and catholyte chamber, and the catholyte and anolyte chambers were separated with an anion-exchange membrane (FAA-3-PK-130, Fumapem). Potassium hydroxide (KOH) solution was used as both the catholyte and anolyte.

Finally, the team evaluated the faradaic efficiencies (FEs) of various products by chronopotentiometry (CP) measurements at 200 mA cm^{-2} coupled with online gas chromatography (GC). They also assessed the stability of the CO_2RR for the experimental sample electrode anodised for 8 hours at 200 mA cm^{-2} in the flow cell electrolyser. Over a period of 12 hours of continuous operation, this electrode sustained an ethylene (C_2H_4) FE above 16%.

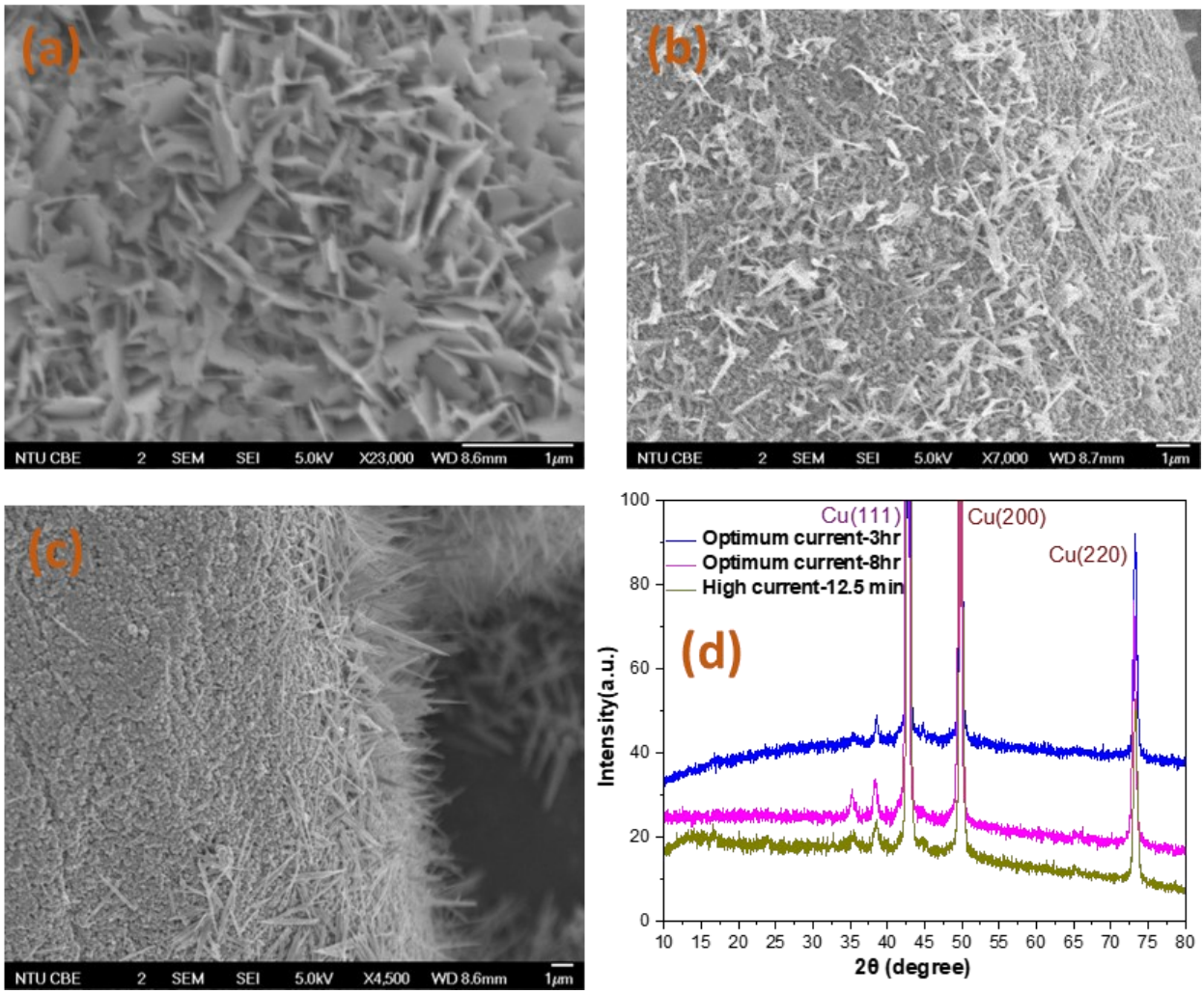


Figure 3.6: Scanning Electron Microscopy (SEM) images of experimental sample electrodes. (a) anodised for 8 hours at the optimum current density, (b) anodised for 1 hour at the optimum current density, and (c) anodised for 12.5 minutes at high current density. (d) X-Ray Diffraction (XRD) spectra of the samples anodised at the optimum current density for 3 and 8 hours, and at a high current density for 12.5 minutes.

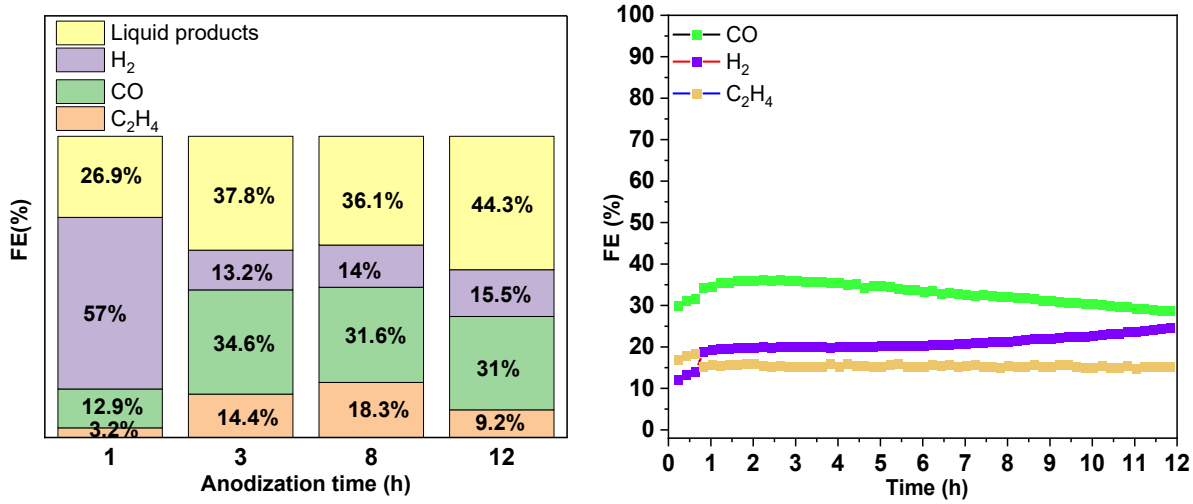


Figure 3.7: The faradaic efficiencies (FEs) for hydrogen (H_2), carbon monoxide (CO), and ethylene (C_2H_4) in the CO_2 reduction reaction (CO2RR) across various experimental sample electrodes subjected to different anodisation durations. Cu mesh anodised for 1 hour predominantly yielded H_2. Extending the anodisation duration to 3 hours decreased the FE of H_2 from 57% to 13.2%, while the FE of C_2H_4 increased from 3.2% to 14.4%. The sample anodised for 8 hours exhibited the highest selectivity toward C_2H_4 (18.3%). However, further increases in anodisation time negatively impacted the performance of the GDE, resulting in a decrease in the FE of C_2H_4 from 18.3% to 9.2%.

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 within ports by building on the success of measuring particulate matter levels with a drone (referred to as UAV), and on characterising and apportioning particulate matter using available sensor data.

During this reporting period, the team targeted potential pollutants emitted from bunkering activities. A comparison of ammonia and methanol sensors was conducted, considering various options including handheld devices and standalone sensors (i.e., low-cost sensor kits), to assess their versatility and compatibility with drones. Ultimately, the team selected and purchased methanol (SKZ 1050, SKZ Inc.) and ammonia (Dräger X -am 8000) sensors for installation on a UAV. The measurement platform was developed utilising a DJI M600 Pro aerial device (DJI Technology Inc.). Additionally, a literature review was conducted to identify potential factors that could impact measurement accuracy, such as drone downwash, flying patterns and wind conditions.

In July 2023, the team participated in a methanol bunkering trial organised by the Maritime & Port Authority of Singapore (MPA), during which measurements were obtained using a UAV. During the methanol bunkering trial, the UAV demonstrated its capability to obtain measurements from extremely close quarters during a potential leaking event with fewer restrictions and safety concerns compared to commonly used measurement techniques, such as using handheld or mounted sensors. Throughout the entire measurement period, no leaks were detected, i.e., the measurable concentration of methanol remained at zero.

The team also investigated additional sensors related to urban emissions and/or global warming, including nitrogen oxides (e.g., NO, NO_2, N_2O), sulphur oxides (e.g., SO_2), volatile organic compounds (VOCs), and environmental data sen-

Figure 4.1 (a): CARES's drone with attached payload (methanol and ammonia sensors).

Figure 4.1 (b): CARES's drone on a test flight during a methanol bunkering trial conducted on 27 July 2023 in Singapore.

sors (e.g., temperature, humidity, wind speed, and wind direction). The measurement data from these sensors could be used for developing and calibrating atmospheric dispersion models.

The team completed the pre-processing of the time series measurement data obtained from the AQMesh sensor system between the years 2020-2023. During the measurement period, the average relative humidity (RH) was reported as 85.3±7.4% and the average temperature was reported as 28.4±2.7°C, both comparable to the average RH and temperature reported in Singapore. The average concentrations of nitric oxide (NO), nitrogen dioxide (NO_2), ozone (O_3), and carbon monoxide (CO) were reported as 21.7±20.1 ppb, 35.0±12.0 ppb, 10.9±7.9 ppb, and 364±94 ppb, respectively. The average carbon dioxide (CO_2) concentration was reported as 532±128 ppm and the average particulate matter (PM) concentrations for PM_1, $PM_{2.5}$, and PM_{10} were reported as 7.8±5.4 µg/m^3, 9.4±6.4 µg/m^3, and 11.8±7.9 µg/m^3, respectively. PM_1 and $PM_{2.5}$ accounted for more than 66% and 80% of the total PM mass, respectively, suggesting the importance of investigating submicron particles. Figure 4.2 shows box plots of $PM_{2.5}$ concentrations, separated by each COVID phase as described in Table 1. No significant differences were observed for $PM_{2.5}$ between the circuit breaker (CB), COVID phases (P2, P3, and P2_2) and the endemic phase (End).

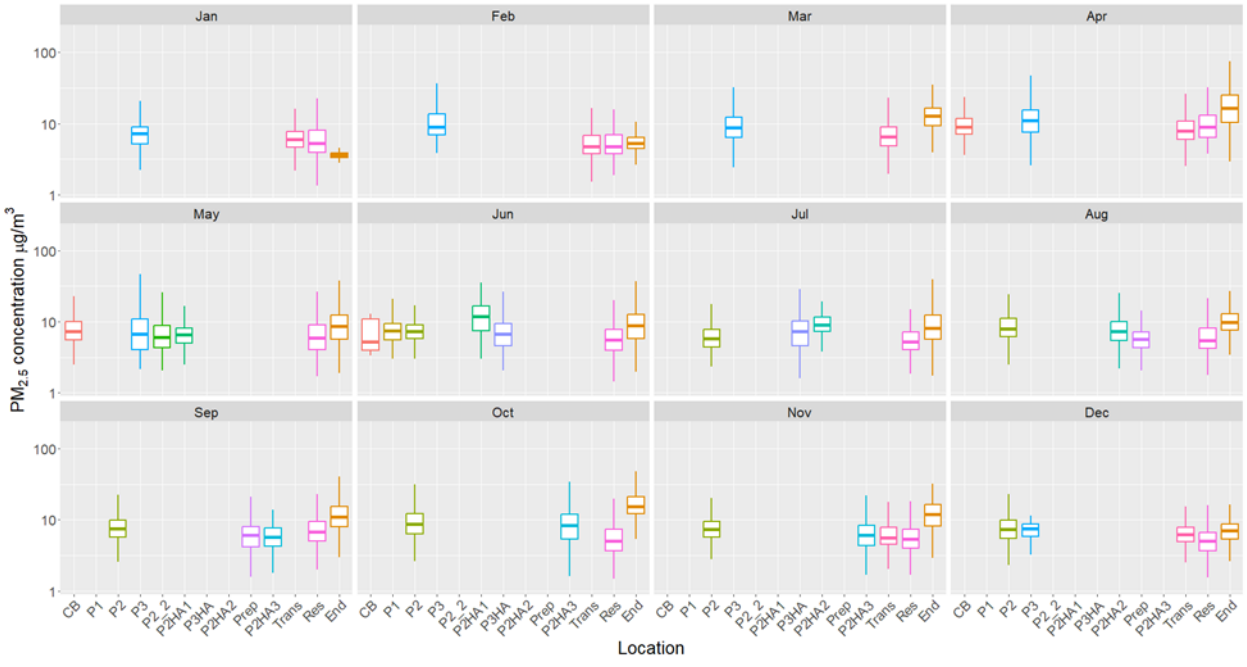


Figure 4.2: Monthly comparison of $PM_{2.5}$ concentration measured by the AQMesh sensor system.

Table 1: COVID phases in Singapore.

Phase	Start Date	End Date	Acronym
Circuit Breaker	4/7/2020	6/1/2020	CB
Phase 1	6/2/2020	6/18/2020	P1
Phase 2	6/19/2020	12/27/2020	P2
Phase 3	12/28/2020	5/7/2021	P3
Phase 2	5/8/2021	5/15/2021	P2_2
Phase 2 heightened alert	5/16/2021	6/13/2021	P2HA1
Phase 3 heightened alert	6/14/2021	7/21/2021	P3HA
Phase 2 heightened alert	7/22/2021	8/9/2021	P2HA2
Preparatory Stage of Transition	8/10/2021	9/26/2021	Prep
Phase 2 heightened alert	9/27/2021	11/21/2021	P2HA3
Transition Phase	11/22/2021	4/25/2022	Trans
Resilient Phase	4/26/2022	2/12/2023	Res
Endemic Phase	2/13/2023	now	End

Using a Non-Parametric Wind Regression (NWR) analysis tool, a brief wind analysis was also conducted with the timeseries measurement data obtained from the AQMesh sensor system, as shown in Figure 4.3. NWR analysis requires a sufficient number of data points (typically more than 1,000 data points) to generate reliable results. However, over the course of the measurement period using the AQMesh sensor system, there were some phases of data loss, resulting in only 200 data points being collected during the CB period. Although the dataset was not sufficient to produce conclusive results, the NWR analysis provided potential hotspots of the species of interest. For instance, during the CB period, $PM_{2.5}$ sources were estimated to be coming from the southwest direction, particularly when wind speeds were between 0-8 m/s. This suggests potential significant contributions of $PM_{2.5}$ from sources located in Jurong Island, situated southwest from the monitoring location.

The team also extended The World Avatar (TWA) to assess how emissions from shipping activities may affect air quality in Singapore, using an atmospheric dispersion modelling system (AERMOD). Multiple heterogeneous datasets from various domains, such as real-time information about ships and weather conditions as well as building geometries, were integrated into the knowledge graph, serving as input parameters to AERMOD. The emission concentration values obtained from the AERMOD dispersion modelling results are also calibrated with actual measurement data. The team is in the process of comparing the AERMOD dispersion modelling results with the measurement data obtained from the AQMesh sensor system.

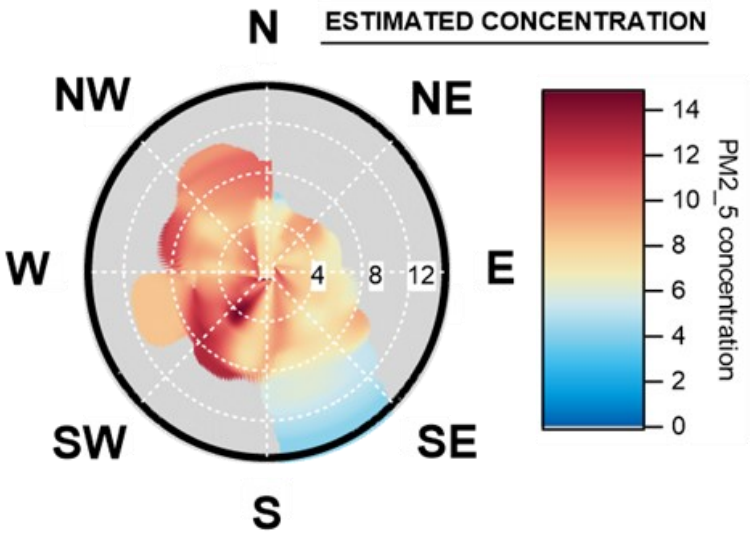


Figure 4.3: Non-Parametric Wind Regression (NWR) analysis of $PM_{2.5}$ sources during the circuit breaker period using timeseries measurement data obtained from the AQMesh sensor system.

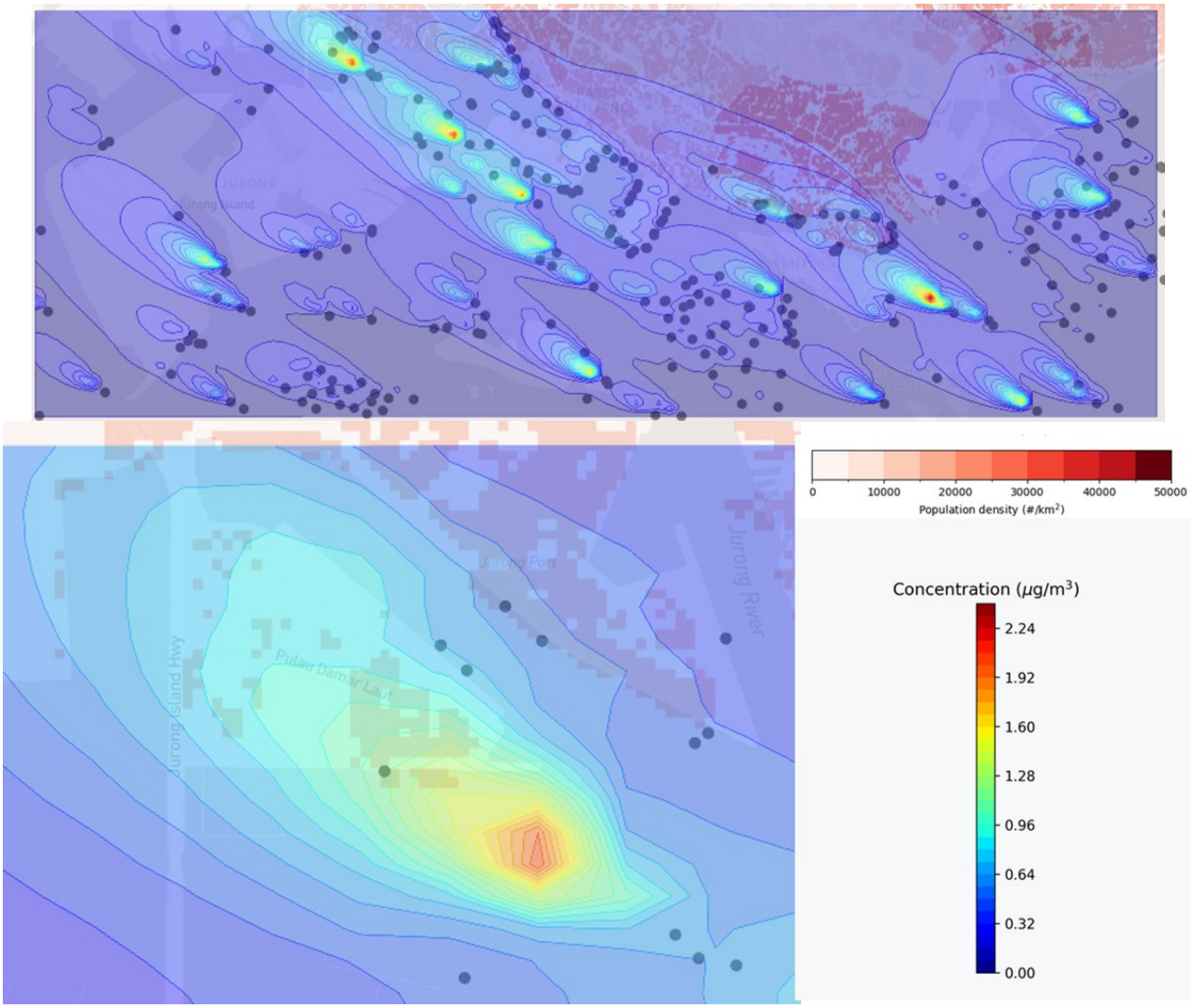


Figure 4.4: Dispersion profile of emissions from ships simulated by an atmospheric dispersion modelling system (AERMOD), overlaid on population density.

Dr Mutian MA (Research Fellow, CARES) investigated how sensors were selected to meet the requirement for ammonia leaking and ammonia engine emission detection. A sampling system was designed with a DJI M600 Pro drone to address the challenging measurement conditions. The sampling system was prepared for the coming ammonia ship test conducted by the Maritime & Port Authority of Singapore (MPA) including bunkering and commissioning practices.

Pollution data collected from the AQMesh (Environmental Instruments Ltd) were based on the timeseries of individual gas pollutant including nitric oxide (NO), nitrogen dioxide (NO_2), ozone (O_3), and carbon monoxide (CO), carbon dioxide (CO_2), and particulate pollutants including PM_1, $PM_{2.5}$, and PM_{10}. Advanced techniques including source apportionment analysis (positive matrix factorization, PMF), and non-parametric wind regression (NWR) analysis that coupled with wind data were performed. Results of the advanced analyses are shown in Figures 4.3 and 4.5. Although AQMesh data cannot provide conclusive evidence to separate sources, both advanced analyses laid the foundation for further collaboration with the World Avatar™ virtual sensor project and potential source apportionment practice using additional data from NUS Environmental Research Institute.

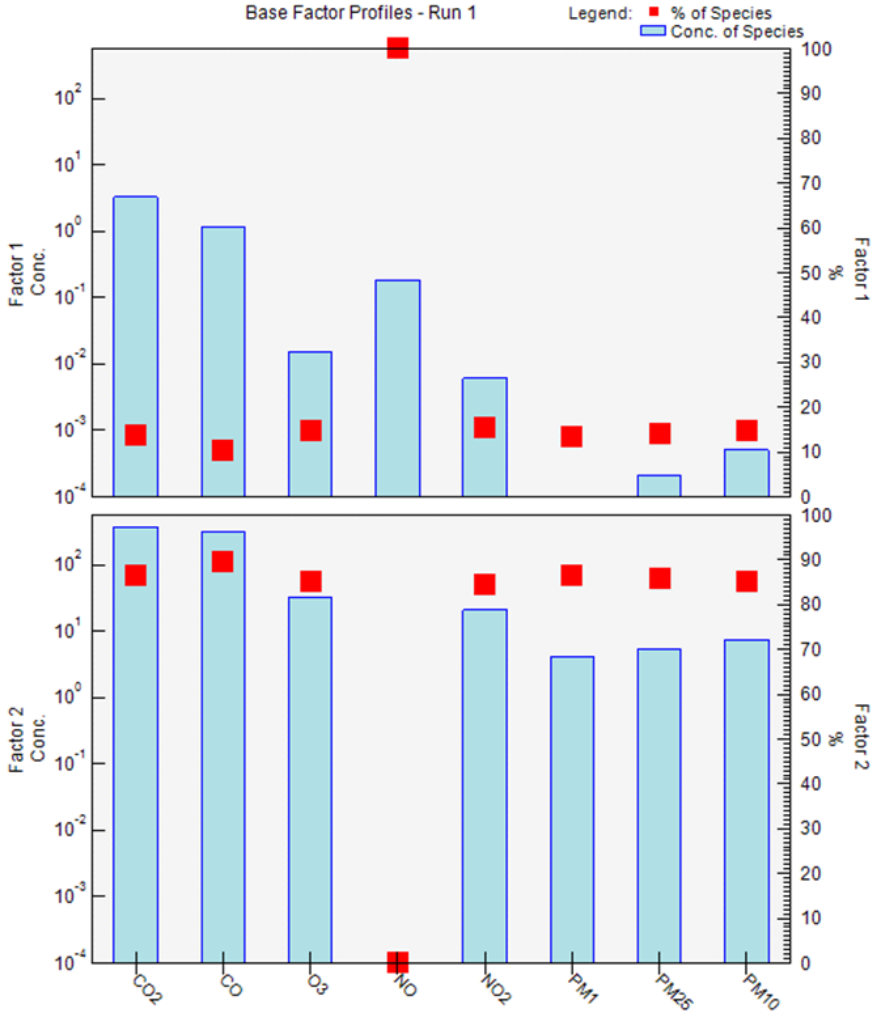


Figure 4.5: Positive matrix factorization (PMF) analysis on source apportionment during COVID circuit breaker period. 2 factors were identified while both are generic factors (i.e., not distinct enough to pinpoint specific source).

Dr Mutian MA

Dr Yong XU (Research Fellow, CARES) focused his research on methanol which has been gaining popularity in recent years, particularly for marine engines. In Singapore, the Maritime Singapore Decarbonisation Blueprint [1] considers methanol as a strong long-term fuel candidate for international shipping. This is because methanol has many advantages, including low cetane number (~3), low net carbon and pollutant emissions. In addition, the current methanol production and transportation infrastructures makes the application of methanol feasible, especially for marine power systems. Modelling of dual-fuel experiments at engine-like conditions has started with the CFD code CONVERGE and the Doubly-Conditioned Moment Closure (DCMC) sub-grid combustion model.

Under the guidance of **Prof Epaminondas MASTORAKOS (PI, CARES)**, Dr Xu conducted Numerical Simulation of Diesel-Methanol Combustion in Constant Volume Chamber. He found that most of the experimental studies focued on the engine performance and engine-out emissions. However the autoignition and flame propagation inside the combustion chamber were not well understood.

Therefore, Dr Xu started with the non-premixed combustion in a constant volume chamber. This project follows two steps: initially, he simulates 0D Diesel-Methanol Combustion (DCMC), where xi1 represents Diesel (modeled as 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. Subsequently, he will run CONVERGE for this 3D problem, including native CONVERGE with no turbulent combustion model (other than the right chemistry), or with LES.

CN3: Lifecycle and system-level studies of marine decarbonisation

Prof Epaminondas MASTORAKOS (CAM)

Dr Li Chin LAW (Research Fellow, CARES) has been working on the continuation of the onboard pre-combustion carbon capture and storage (CCS) research utilising the internal combustion engine (ICE) as an energy converter. An exploration into the gas turbine (GT) as a substitute for the ICE was conducted. A GT with higher exhaust temperature provides a significant amount of high-grade heat for waste heat integration. In this study, various waste heat utilisation schemes were simulated in Aspen HYSYS for closed-loop analysis. It was determined that the effective utilisation of high-grade heat from the GT exhaust and intermediate processes (downstream of the steam methane reformer, SMR) is essential for enhancing overall energy efficiency and carbon capture rates. These findings support the long-term viability of integrating pre-combustion CCS with combined-cycle gas turbine (CCGT) system as a strategy for decarbonisation, aligning with emissions regulations.

In the realm of low carbon ship design fuelled by alternative fuels such as hydrogen, ammonia, methanol, and biofuels, various factors come into play beyond just fuel properties. Considerations such as voyage patterns, ship characteristics and external elements like weather condition and sea state are equally important. In the current model, voyage speed, deadweight and voyage distance were correlated with ship performance, which is measured by metrics such as cargo attainment rate (CAR) and carbon intensity (CII). Future research should focus to develop a more comprehensive multi-parameters model, which would allow for the correlation of additional factors impacting low carbon ship performance.

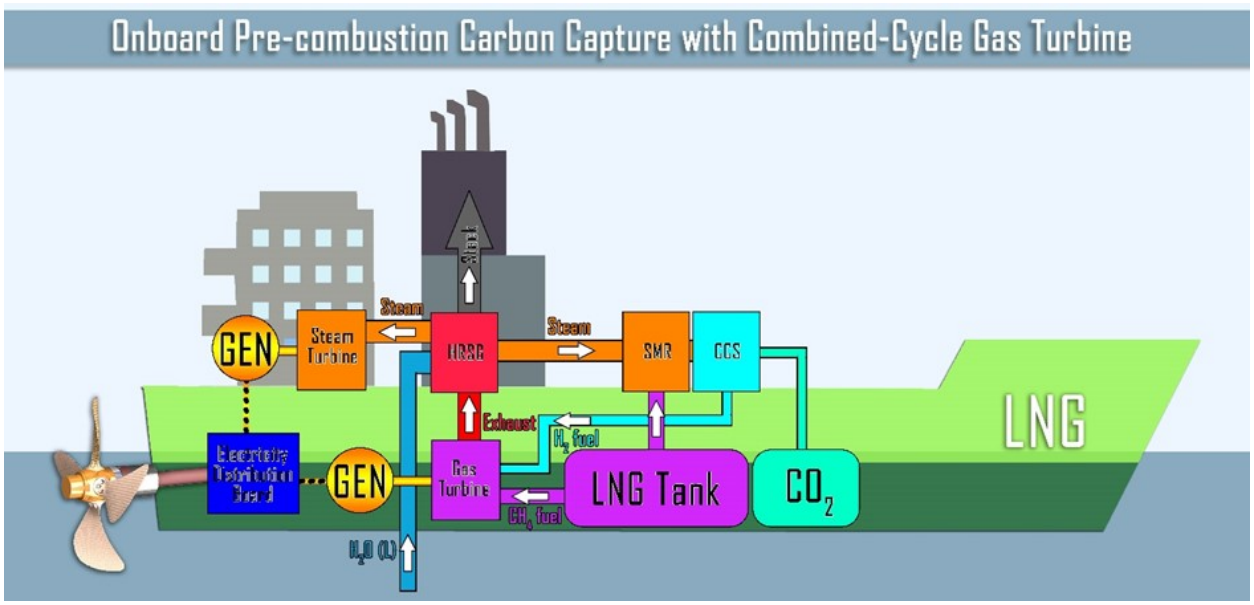


Figure 4.6: A block diagram of the ship-based integrated system composed of CCGT, SMR, and pre-combustion CCS systems.

Dr Li Chin LAW

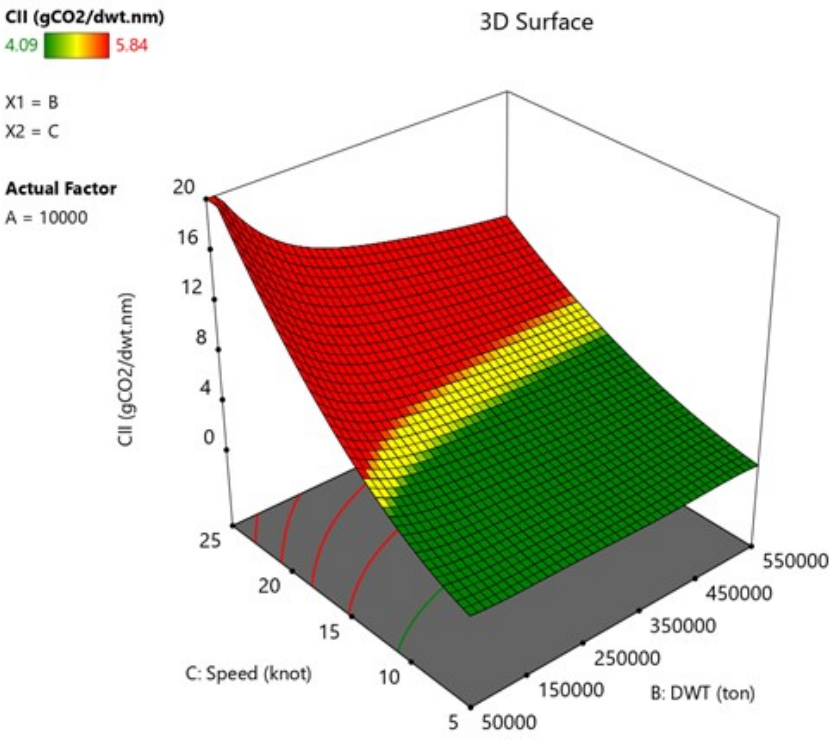


Figure 4.7: The chart illustrates the changes in CII with voyage speed and ship deadweight.

Dr Li Chin LAW

Before initiating any action to improve a ship's carbon rating, it is paramount to visualise and project the greenhouse gas intensities relative to the decarbonisation timeframes, so that timely interventions could be implemented. To facilitate this process, a CII and FuelEU Maritime calculator has been developed and shared publicly on the webpage, www.emi-cast.com/calculator. This calculator allows the visualisation on the difference of greenhouse gas emissions with fuel, ship and voyage characteristics.

Figure 4.8: Researcher's illustration of the EMICAST calculator

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 researching ammonia and its potential as a marine fuel. Its use raises concerns due to its toxicity which can lead to hazardous situations in the event of leaks. Compared to other alternative fuels, ensuring safety with ammonia presents a significant challenge. Given that ship-to-ship bunkering is a crucial activity in the maritime sector, it is essential to study the consequences of potential ammonia leaks. Dr Liu used Computational Fluid Dynamics (CFD) to simulate various ammonia leakage scenarios during ship-to-ship bunkering. As a first step in the validation of the numerical set-up, simulation of controlled experiments was performed and the accuracy was satisfactory. For the ship-to-ship bunkering, leaks at various orientations relative to the wind, and of the wind orientation relative to the ships, were considered.

The results show that the atmospheric dispersion of ammonia is greatly affected by obstacles like the superstructure and the hull of the vessel in the near field with the effect becoming weaker at the far field. The accuracy of the usual Gaussian plume models for the first few hundred meters from the release is limited due to the complex streamline pattern in the near field and the extra turbulence induced by the wakes of the hull and the superstructure that invalidate the assumptions behind the Gaussian plume theory. A consequence analysis reveals that an upward leakage induces a larger risk zone where people could experience irreversible or long-lasting adverse health effects. In the forward and horizontal leakage scenarios, personnel are more likely to be exposed to life-threatening concentrations, while a vertical leakage in a crosswind configuration causes a lethal area that covers tens of meters on deck. The results suggest that risk analyses of ship-to-ship ammonia bunkering must be done with great attention to the exact location of the transfer pipe relative to the ship and for all possi-

ble wind orientations. It is recommended that simulations like the present ones are carried out for every ammonia-fuelled ship before such activities are certified as safe due to very wide variety of possible dispersion patterns and the fact that the usual Gaussian dispersion models based on point source and uni-directional flow, which are often used in risk analysis, are almost irrelevant at the ship scale.

Here, two representative figures are provided. Figure 4.9 illustrates the schematic diagram for ship-to-ship ammonia bunkering operations, while Figure 4.10 shows the ammonia mass fraction in regions close to ammonia leakage source at X, Y and Z slices for different scenarios. Dr Liu and his co-authors have prepared a manuscript based on this research and submitted it to *Ocean Engineering* for publication.

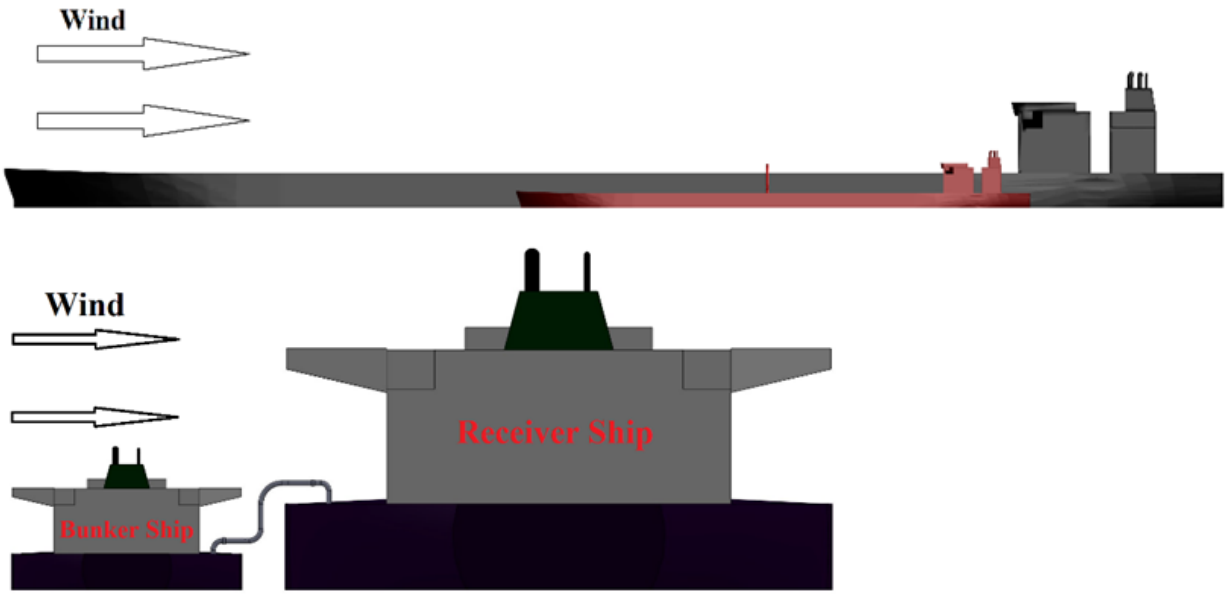


Figure 4.9: Schematic diagram for ship-to-ship ammonia bunkering operations: (a) the parallel wind case and (b) the crosswind case.

Dr Yangyang LIU

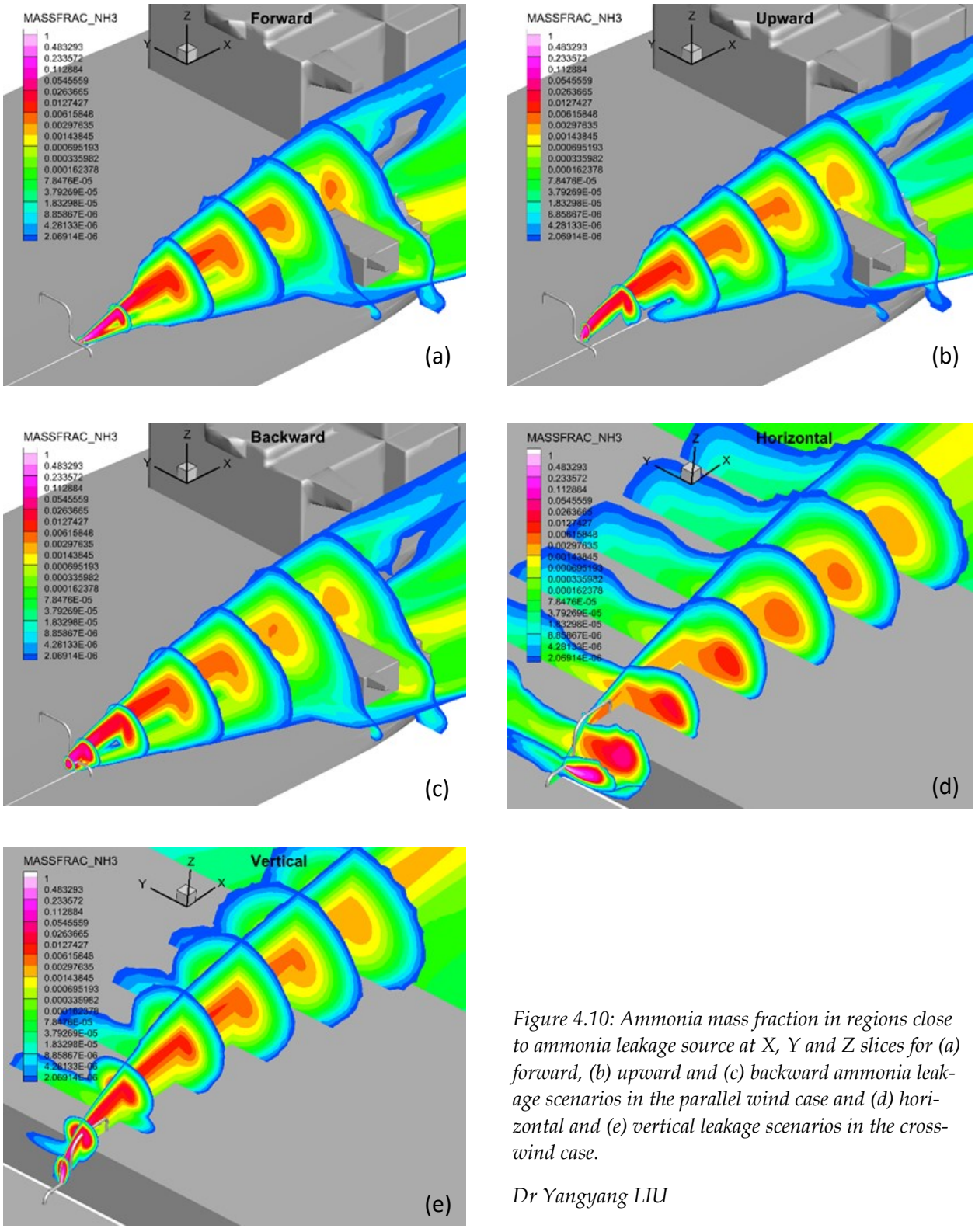


Figure 4.10: Ammonia mass fraction in regions close to ammonia leakage source at X, Y and Z slices for (a) forward, (b) upward and (c) backward ammonia leakage scenarios in the parallel wind case and (d) horizontal and (e) vertical leakage scenarios in the cross-wind case.

Dr Yangyang LIU

Dr Ramesh KOLLURU (Research Fellow, CARES) used Converge Computational Fluid Dynamics (CFD) software to investigate how a ship performs under different wind conditions: headwind, inclined wind, and crosswind. Additionally, a comparative analysis was carried out among these scenarios using a Gaussian plume model, which involved the assessment of various dispersion coefficient evaluation models. This comparison aimed to gauge the accuracy of the Gaussian plume model in predicting the dispersion of pollutants. In Figure 4.11, the streamline patterns for the three simulated scenarios are depicted. Notably, the presence of recirculation zones in the wake region is observed, stretching up to 1.5 times the width of the ship. These recirculation zones are crucial as they significantly impact the mixing processes within this area. It's worth noting that turbulence induced by the ship's wake plays a dominant role in enhancing mixing in these zones, influencing the dispersion of pollutants and overall atmospheric dynamics.

Figure 4.12 depicts the normalised contours of passive scalar at different planes for all three scenarios. It can be observed from Figure 4.12 that in the headwind and crosswind cases, the plume evolution is symmetric. In the inclined case, the evolution is asymmetric. The asymmetric nature of the plume is attributed to the macromixing developed behind the ship.

This work emphasises the importance of considering different dispersion models and their sensitivity to atmospheric conditions to understand passive scalar emissions comprehensively.

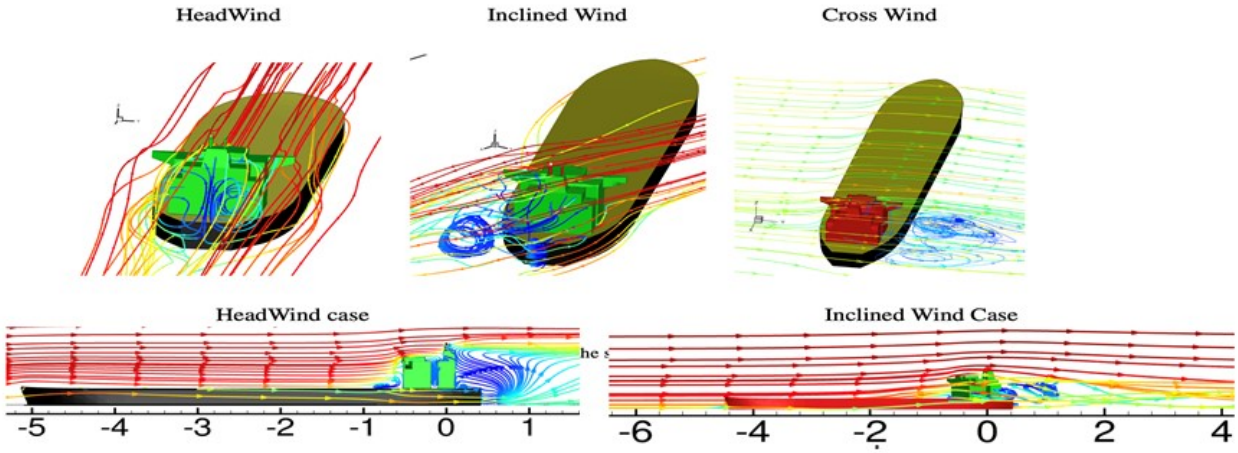


Figure 4.11: Streamlines over ship for all three wind conditions. The model is generated in a 3D plane (X, Y, and Z). The spatial coordinates are in metres.

Dr Ramesh KOLLURU

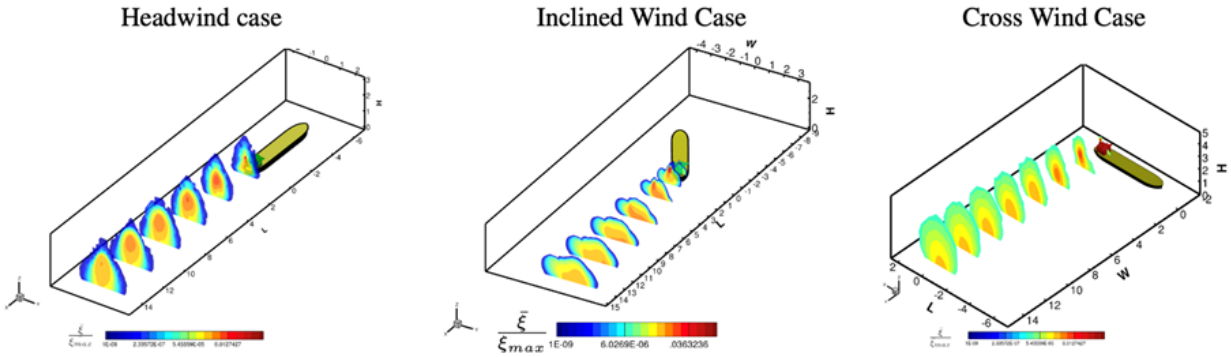


Figure 4.12: Evolution of passive scalar at various planes in the wake region.

Dr Ramesh KOLLURU

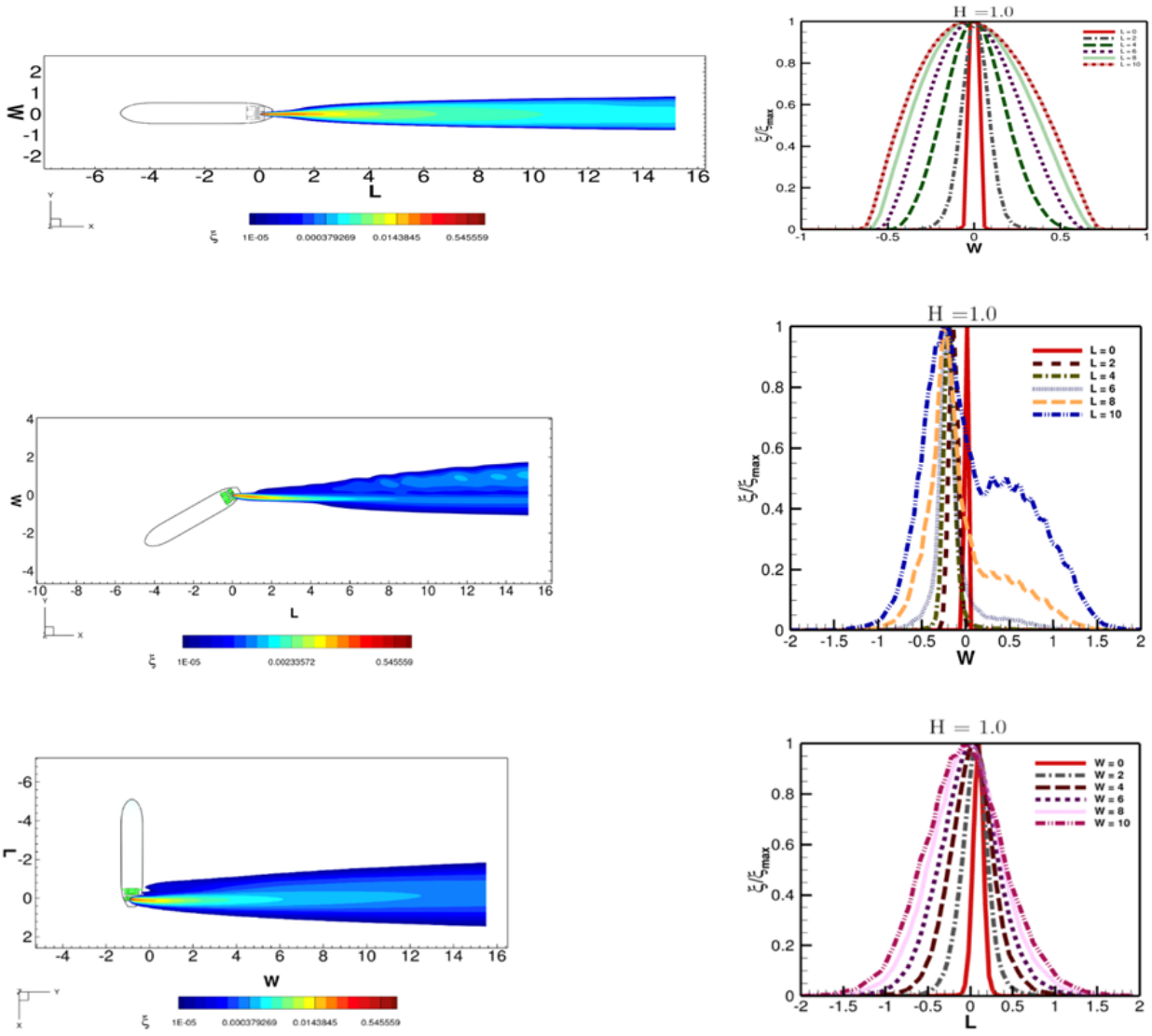


Figure 4.13: Gaussian profiles of normalised passive scalar plotted at different distances from the main stack of the ship, all normalised at a nondimensionalised height of H = 1.0. (top) Headwind, (middle) Inclined, and (bottom) Cross wind.

Dr Ramesh KOLLURU

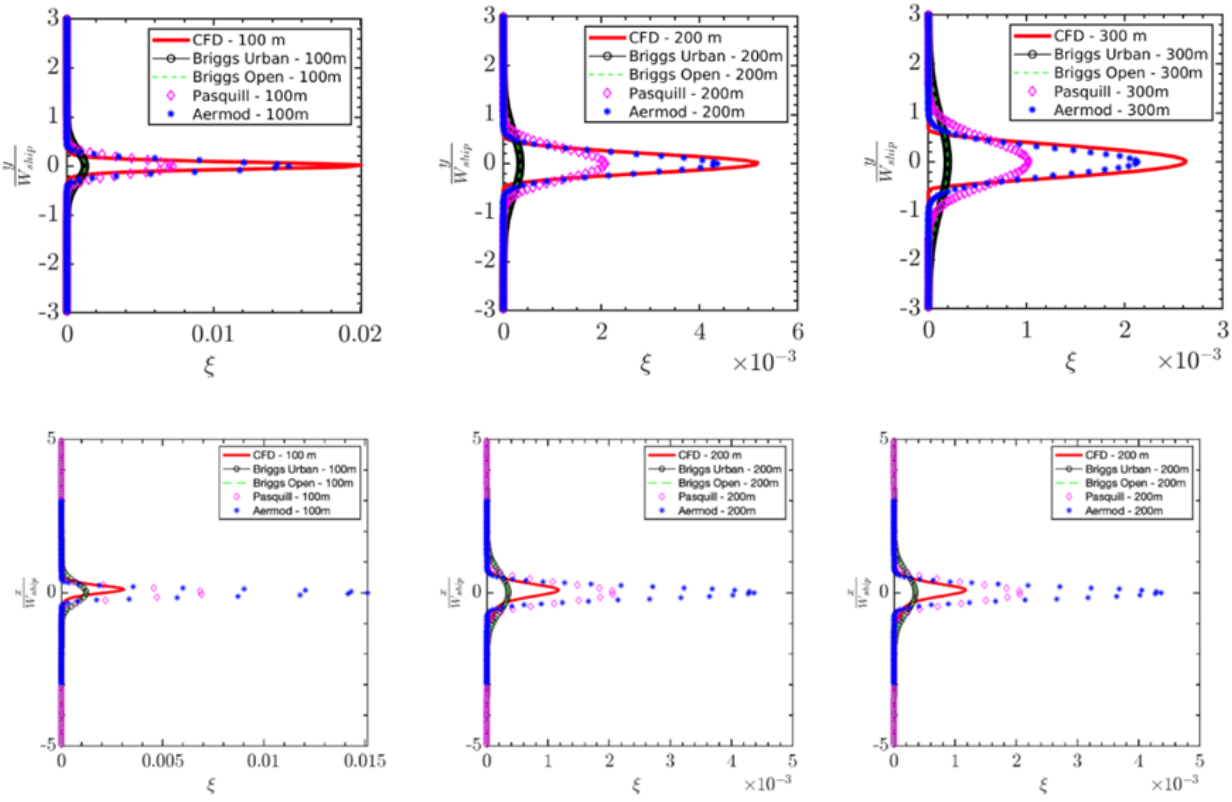


Figure 4.14: Comparison between Gaussian plume model and CFD for (top) Headwind and (bottom) Cross wind at various distances.

Dr Ramesh KOLLURU

CN14: Alternative marine fuel engine modelling

Prof Epaminondas MASTORAKOS (CAM)

Dr B HARIKRISHNAN (Research Fellow, CARES) has been testing the newly developed solver **dcmcConverge**, which combines the CFD solver Converge with 3D doubly conditional moment closure (DCMC). It is an advanced turbulent combustion closure. Large-eddy simulation (LES) is chosen as the turbulence model. Dr Harikrishnan presented this work at the AIAA SciTech Forum 2024 by studying the dual fuel turbulent jet-ignition (TJI) problem in a constant volume chamber.

The researcher performed **0D-DCMC** simulations for Ammonia with Decane. Mixture fraction ξ is defined as 0 at the NH_3/air mixture and 1 at the $C_{10}H_{22}$/air mixture. The progress variable defined with the mass fractions of CO_2, CO, H_2 and H_2O. Mechanism by Tay et al. 2017 [2] is used for this case. It has 80 species and 374 reactions.

Currently, the researcher is analysing the dual-fuel swirl flame with Heptane as liquid fuel in the presence of CH_4/air gaseous mixture. The equivalence ratio of CH_4 is under the low flammability limit (LFL). The capability of **dcmcConverge** will be demonstrated by simulating the flame structure and global extinction behaviour in the presence of different fuels. As the first step, the cold flow is simulated in RANS and LES sequential manner. Then the cold spray flow is simulated to stabilise the flow and to tune the spray parameters respectively.

For the next phase, the dual-fuel spray flame will be simulated and validated against the experiments. Also, the SINTEF sequential combustor will be simulated and validated against the experiment in its ability to capture the emission characteristics.

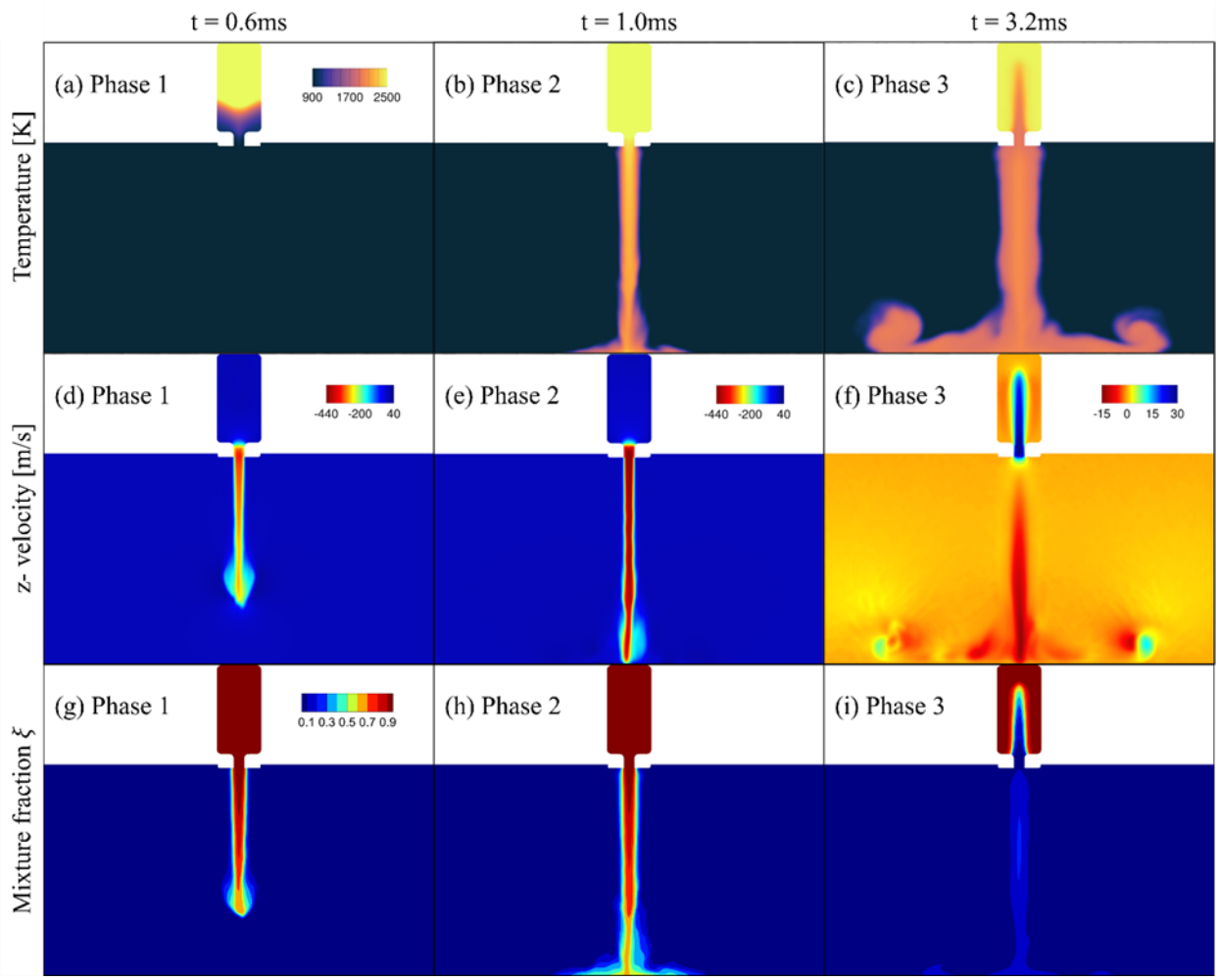


Figure 4.15: Contour plot of the physical field variables for the TJI problem.

Dr B HARIKRISHNAN

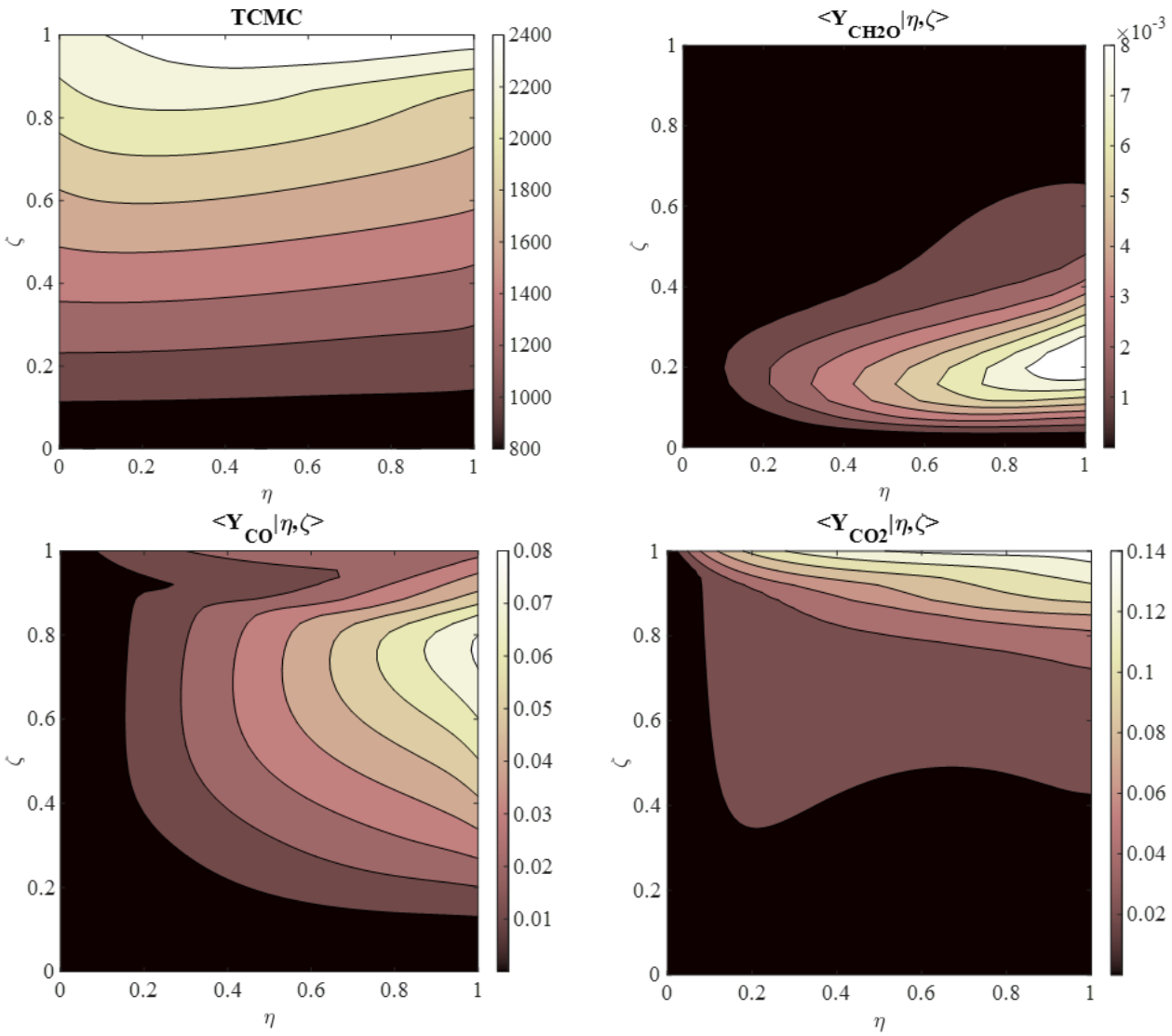


Figure 4.16: Conditional variables in the conserved scalar space.

Dr B HARIKRISHNAN

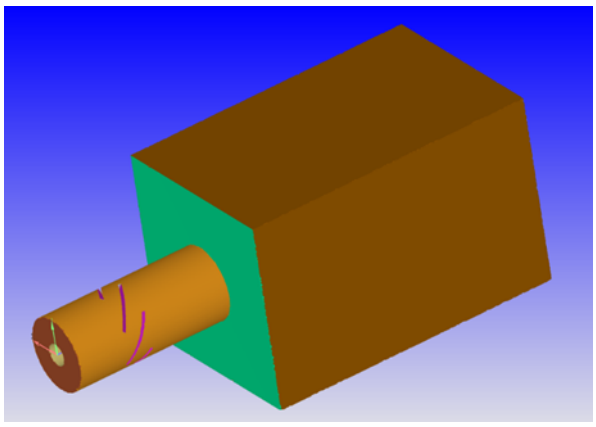


Figure 4.17: Geometry for the Cambridge Swirl burner.

Dr B HARIKRISHNAN

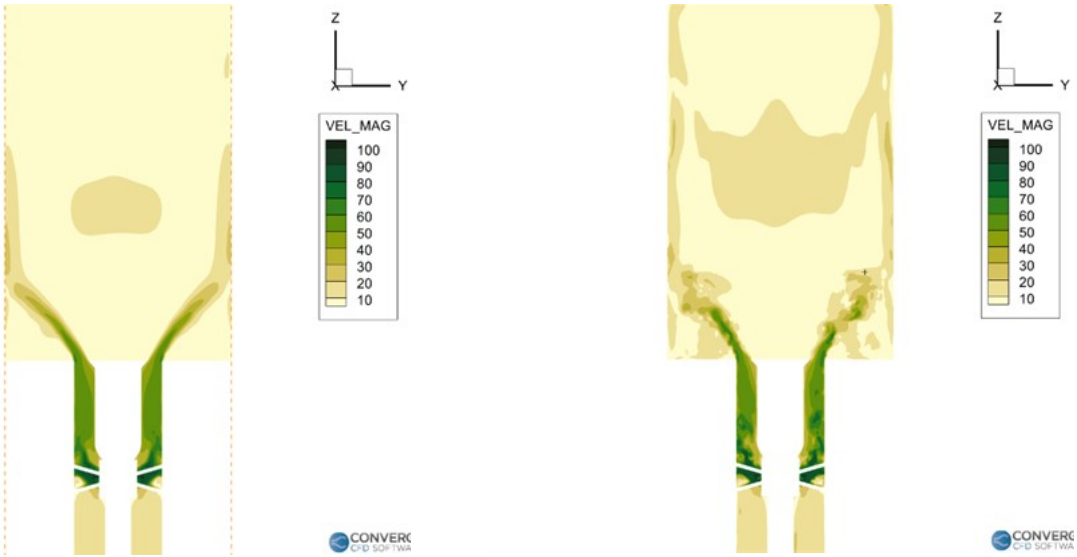


Figure 4.18: RANS (left) and LES (right) simulations of the cold flow.

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) is working on the development and assessment of liquid natural gas (LNG) and Liquid Hydrogen (LH_2) cold utilisation strategies for Singapore. The potential import of LH_2 to tropical countries such as Singapore in its strides to develop a hydrogen economy will bring an available high-grade cold energy content (at -253 ^oC) that far exceeds the current LNG cold energy content (at -162°C). LH_2 can be subject to Cold Energy Storage using Phase Change Materials (PCMs) as it can be more efficiently exploited for various utilisation opportunities.

In the context of LNG cold utilisation, Dr Ayachi's work in the reporting period consists of extending the baseline model and developing integrated process designs that involve i) different cold utilisation purposes (carbon capture at solid/gaseous state vs. CO_2 liquefaction for vessel transportation vs. combined carbon capture and liquefaction) and ii) different carbon capture methodologies including pre-combustion, post-combustion, and oxy-combustion technologies. For each integrated process design, heat and mass balances are obtained by means of steady-state thermodynamic model developed through Aspen Plus V10 simulator. The results indicate for each integrated process design the consequent annual CO_2 removal, the required consumables (e.g. organic chemicals, gases, etc.), the minimum required energy loads, the potential by-products, and the impact of the strategy on annual LNG-based electricity production. As a next step, techno-economic assessment tools would enhance the comparative analysis and help to identify the appropriate integrated process design to meet energy-saving strategies and environmentally friendly objectives.

In the context of LH_2 cold utilisation, Dr Ayachi developed integrated process designs for various utilisation opportunities. In particular, cryogenic cogeneration can be considered as a standalone process for the utilisation of the high-grade cold energy from LH_2 regasification as it can be combined with other utilisation opportunities including process cooling, gas production, and carbon capture. The results have shown that by proposing and optimising specific layouts of cryo-cogeneration cycles depending on the use case, it is possible to achieve high cogeneration efficiencies of up to 61%. This also shows that the investigated cryo-cogeneration processes appear to be promising cost-effective solutions as they get close to the highest performance achieved by a helium Brayton cycle. As a next step, the assessment will include Exergy Analysis, which would help to identify areas of improvement. The assessment will cover novel integrated process designs involving cascading cryo-cogeneration which not only appears advantageous in terms of performance enhancement but could also represent a substantial engineering solution to reduce the impact related to the very large temperature difference in the heat exchangers.

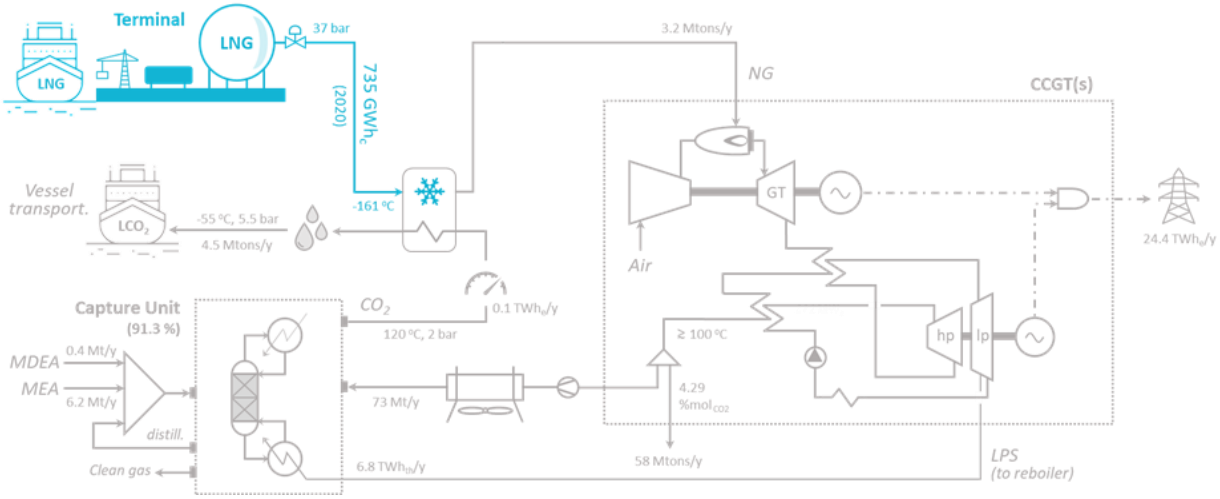


Figure 4.19: Example of integrated process design involving LNG cold utilisation and a post-combustion process for carbon capture

Dr Mohamed Fadhel AYACHI

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[2] Tay KL, Yang W, Li J, Zhou D, Yu W, Zhao F, Chou SK, Mohan B. " Numerical investigation on the combustion and emissions of a kerosene-diesel fueled compression ignition engine assisted by ammonia fumigation". Applied Energy 2017. 204:1476-1488. DOI: 10.1016/j.apenergy.2017.03.100

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 solar business models. A numerical study is currently ongoing to expand the analytical results and test different scenarios based on publicly available market data. The first manuscript is being prepared for submission, to be followed by a second manuscript that incorporates hybrid pricing models for third-party ownership.

Dr Yan WANG (Research Fellow, NTU has collaborated with **Prof S. VISWANATHAN (PI, NTU)** on a working paper titled "Sustainability Reporting Quality and Carbon Emissions Reduction: the Role of Chief Sustainability Officer." Dr Wang is finalising the manuscript for submission.

Prof Viswanathan, Dr Martin, and Dr Wang are currently working on a project to analyse carbon tax implementation and its downstream impact on the price of commodities. Dr Wang has compiled a comprehensive review of carbon tax/ quota policies worldwide. In addition, she has collected data on shipping routes and prices for several commodities. Dr Martin has conducted an initial study assessing the potential impact of carbon taxes on inducing clean technology adoption in the maritime sector and is looking towards a similar study involving the oil and gas sector.

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. Specifically, the project will focus on Covalent Organic Frameworks (COFs), a versatile subclass of porous polymeric materials that demonstrate exceptional potential in diverse fields such as printable electronics, gas storage (particularly for carbon and water vapour capture), and broader environmental remediation efforts. Using this approach, high value molecules that are previously not recorded in the literature can be proposed at a faster rate, and the proposed molecules could potentially be automatically synthesised using the next generation laboratory.

During this reporting period, the team developed a computational agent, called the COF Construction Agent, and its associated method to address a critical need in COF design: the ability to predict and optimise crucial physical properties of COFs such as porosity, electronic structure, available surface area, and stacking configurations. These properties are essential for tailoring COFs to specific applications. The COF Construction Agent, a Reticular Construction Agent, is designed to facilitate the design and optimisation of COFs. It streamlines the design process through its capabilities in subunit construction, stacking, and optimisation. Integration of this COF Construction Agent within The World Avatar (TWA) enables the systematic generation of new COFs directly from accumulated knowledge within the knowledge graph, accelerating the discovery of materials with tailored properties.

The COF Construction Agent leverages the Automatic Topological Generator for Framework Structures (AuToGraFS) library, which employs graph-theoretical algorithms to generate and optimise COF structures. The workflow begins with an initialisation of the computational environment and loading relevant COF precursors and building block data. It then utilises reticular chemistry principles to model COFs as graphs, where nodes represent molecular building blocks, and edges denote potential chemical bonds. The COF Construction Agent then performs subunit construction by leveraging a chemical ontology to define allowable subunits and uses geometric transformations to ensure correct alignment for integration with AuToGraFS. To accommodate the diverse chemistries involved in COF synthesis, the structural inputs are carefully adjusted for AuToGraFS, and the workflow strategy is adapted based on the specific linkage formation and framework type. This customisation is crucial for generating accurate and realisable COF designs.

While AuToGraFS is a powerful COF generation tool, it often requires precise guidance regarding the choice of building units and the exact nature of the linkages between them. To address this, advanced computational methods were employed in the subunit construction process to streamline subunit selection, assembly, and refinement, while ensuring compatibility with AuToGraFS. This process begins with creating the input files and establishing a tailored computational environment for accurate molecular data processing. The inputs are then transformed into structured formats, facilitating intricate atomic-level manipulations crucial for customising COFs. Following this, the molecular structures

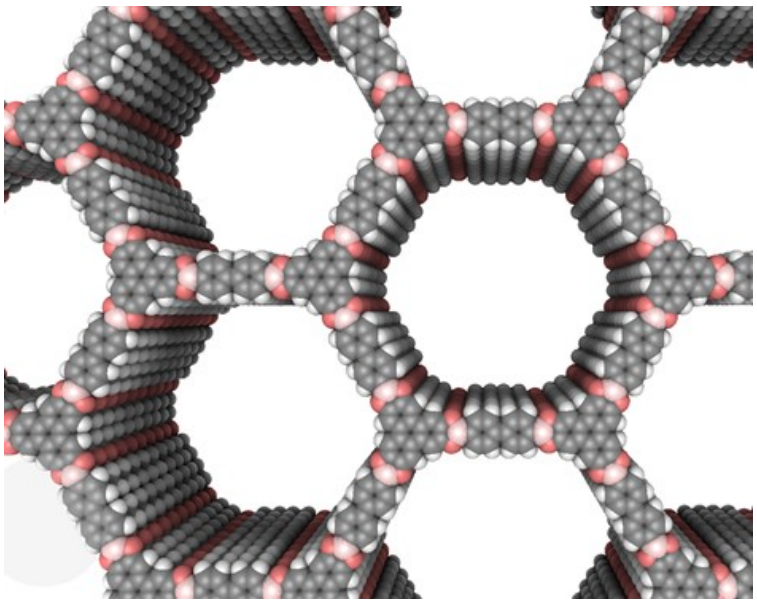


Figure 5.1: Example of an optimised COF structure constructed by the COF Construction Agent.

are carefully modified using advanced algorithms, such as targeted atom replacement and rotation within building units, to ensure correct alignment with the desired COF architecture. Geometric transformations are also used to ensure that atoms are precisely positioned and oriented within the subunits, creating a blueprint for accurate COF construction. Finally, the processed data is reformatted for compatibility with AuToGraFS, ensuring that the constructed COF subunits are ready for computational analysis, optimisation, and performance prediction. By strategically defining bonding patterns and orientations within building blocks, the subunit construction functionality clarifies how AuToGraFS should connect units with simple linear linkages, thereby avoiding any potential design ambiguities.

While AuToGraFS and similar tools are powerful for designing idealised two-dimensional COF structures, understanding how these COFs assemble into layered materials is crucial for comparison to experimental results. In experiments, COFs rarely exist as single layers; instead, interlayer interactions lead to the formation of stacked structures. The specific stacking arrangement (e.g., AA, AB, or other configurations) can significantly influence a COF's measured properties such as porosity, conductivity, and stability. To address this, dedicated methods were incorporated into the COF Construction Agent to extract atomic coordinates and lattice parameters from relevant files, allowing precise geometric manipulations of individual layers. These methods support both AA and AB stacking modes, as well as other potential configurations. This flexibility enables the exploration of different stacking arrangements, helping to bridge the gap between theoretical predictions and experimental observations.

The COF Construction Agent also leverages various techniques to optimise COF properties, aiming for a balance between computational efficiency and the ability to handle the diverse structures encountered in COFs. DFTB+ is a simulation software used for computationally efficient quantum mechanical calculations, focusing on tasks such as structural refinement, electronic property prediction, and binding energy calculations. The team designed the COF Construction Agent to interact with dedicated microservices for DFTB+, and other optimisation tools, creating a modular design that simplifies the workflow and allows researchers to focus on analysis and iterative COF design refinement. When DFTB+ parameters are not readily available, the COF Construction Agent is designed to employ force field (FF) methods for optimisation. Additionally, MolVol calculations are incorporated to assess cavity size and internal pore structure, which are critical factors in applications such as gas storage and separation.

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 is expected 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.

The realisation of self-driving laboratories requires a connection between abstract chemistry knowledge and concrete laboratory hardware for execution. To address this, during this reporting period, the team developed a set of related ontologies aimed at reducing gaps in current semantic representations for chemical digitalisation. These ontologies cover a range of aspects, from high-level research goals (OntoGoal), chemical reactions (OntoReaction), mathematical design of experiments (OntoDoE), to the physical execution of reaction experiments in the laboratory (OntoVapourtec, OntoHPLC, and OntoLab).

For the proof-of-concept, an aldol condensation reaction between benzaldehyde and acetone, catalysed by sodium hydroxide to yield the target product benzylideneacetone, was selected. Benzylideneacetone can be used to treat idiopathic vomiting as an NK-1 receptor inhibitor. Other reported side products of the reaction include dibenzylideneacetone and further condensation products from acetone polymerisation.

The team developed a knowledge graph to connect two similar automated flow chemistry platforms located in Cambridge and Singapore. Each platform consists of two Vapourtec R2 pump modules, one Vapourtec R4 reactor module, and one four-way VICI switching valve. The platform in Cambridge uses a liquid handler to source the input chemicals, while the one in Singapore uses reagent bottles. Upon initiating the experiment, the system is designed to first determine whether the reaction has reached a steady state, after which, the four-way VICI valve is switched to send the chemicals for analysis in the High-performance Liquid Chromatography (HPLC) system. As the platform in Cambridge uses a HPLC analytical equipment from Shimadzu, while the platform in Singapore uses an Agilent 1260 Infinity II system, the team had to develop the analytical method for each HPLC and calibrate it against the product materials.

The dynamic nature of the knowledge graph is achieved by using software agents that realise each step in the iterative design-make-test-analyse (DMTA) workflow and facilitate the flow of information within the knowledge graph. The process begins with the goal derivation stage, where the scientist initiates a goal request. The Reaction Optimisation Goal (ROG) Agent translates this request into a machine-readable statement. This translated request then triggers the Reaction Optimisation Goal Iteration (ROGI) Agent to create tasks for the relevant agents (including the DoE Agent, Schedule Agent, and Post-Processing Agent) to achieve the request initiated by the scientist, according to the DMTA workflow. After each iteration, the ROG Agent utilises the obtained results to determine whether the next iteration should be pursued, by checking if the Pareto front of the multi-objective optimisation problem fulfils the pre-defined goals and whether the resources to continue the next iteration are still available. When necessary, the ROG Agent will make a new request to the ROGI Agent to start a new iteration, thereby forming a self-evolving feedback loop.

The actual experiment conducted using the two self-driving laboratories consisted of an optimisation of the cost-yield objectives involving 65 data points. Throughout the operation, the two self-driving laboratories shared experiment results with each other when proposing new experimental conditions. The real-time collaboration demonstrated faster advancements in the Pareto front, with the highest yield reaching 93%. Since the chemicals used in this study were obtained from different vendors compared to the litera-

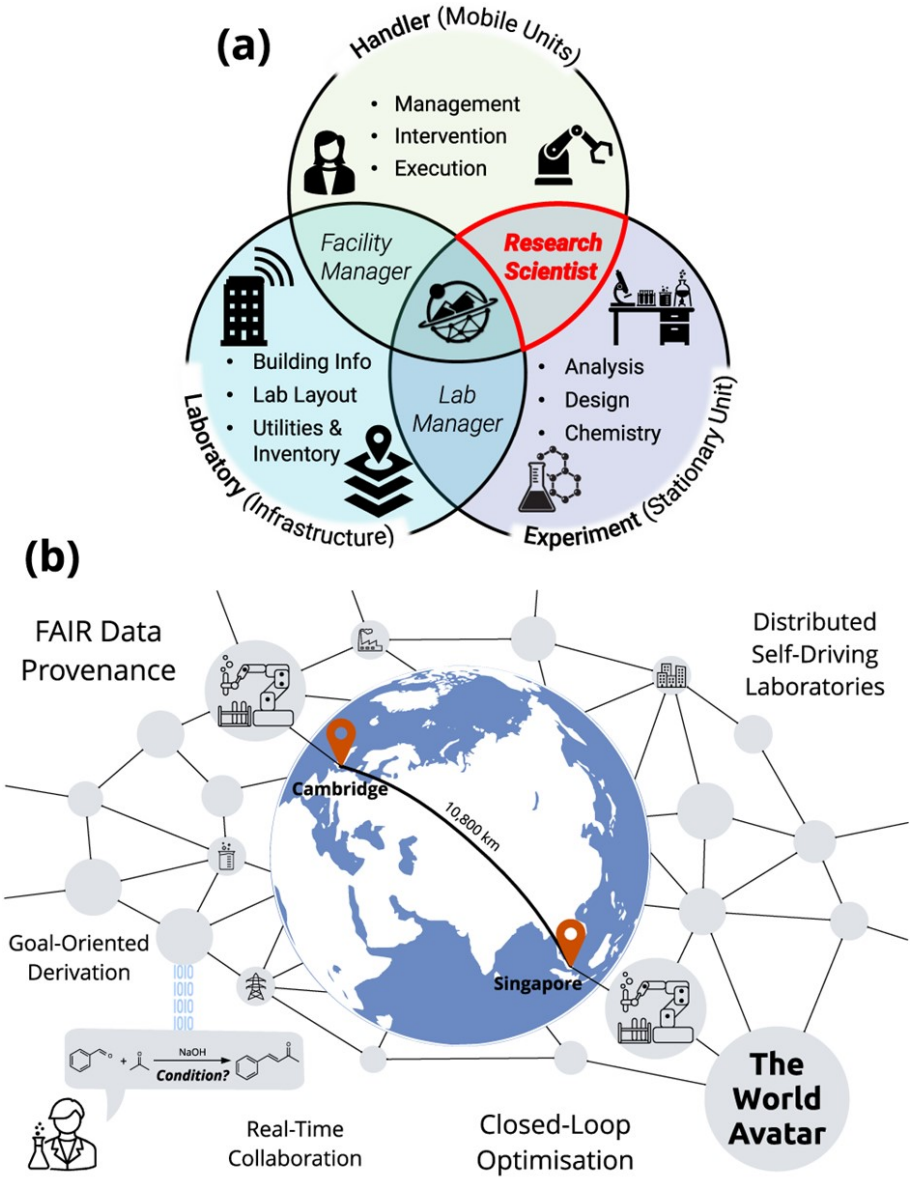


Figure 5.2: (a) An overview of the intertwined aspects of a future chemical research laboratory represented by our Digital Laboratory Framework. (b) Connecting two automated flow chemistry platforms located in Cambridge and Singapore using the dynamic knowledge graph approach.

ture, the cost optimisation results are therefore not directly comparable due to differing prices. Although not considered in the optimisation, the environmental factor and space-time yield were found to highly correlate with the yield objective. The best values obtained from the experiments were 26.17 and 258.175 $g \cdot L^{-1} \cdot h^{-1}$ when scaled to the same benzaldehyde injection volume (5 mL), both of which outperformed results reported in the literature.

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 on addressing various aspects of a typical pharmaceutical laboratory. Specifically, the project will create digitised, automated, and interconnected virtual representations of selected analytical equipment in the CARES Laboratory, such as the Gas Chromatography – Mass Spectrometry (GC-MS) system. This demonstration will showcase the automated transcription of testing and product-quality-relevant process data, effectively reducing the need for manual documentation work. 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 ensures improved quality and compliance by minimising manual errors and variability, as well as facilitating seamless data retrieval and analysis. This, in turn, enables faster and more effective resolution of problems and laboratories can significantly decrease their investigation workloads.

During this reporting period, the team has created tools that enable laboratory users, especially the laboratory manager, to access laboratory information on the go. These tools include various mobile applications, an interactive dashboard based on the Grafana platform, and an Augmented Reality application. These tools integrate both information about the building in which the laboratory is situated and sensor data within the laboratory originating from different sources and vendors, all into one interface for better monitoring and management of the laboratory.

Using the time series data from the laboratory's Building Management System, the team developed an interactive dashboard using the Grafana platform, as shown in Figure 5.3, which displays various parameters such as outdoor weather conditions, indoor laboratory conditions including air flow rates, temperature, humidity, and the electricity usage in the laboratory. The dashboard can be used to monitor the operating conditions of the laboratories and their critical systems such as the Makeup Air Units. This will allow the laboratory manager to analyse energy consump-

Figure 5.3: The CARES Laboratory Grafana dashboard for day-to-day monitoring of the laboratory conditions. It integrates data from a variety of sources, including an outdoor weather station, the laboratory's Building Management System, and an electricity meter to facilitate holistic monitoring of the laboratory operations.

tion patterns and assess the impact of energy saving measures on the laboratory easily. Furthermore, the team developed a Dashboard Agent to automate the creation of the dashboard from various data sources within the knowledge graph, according to user preferences.

The team also developed an Augmented Reality application for real-time laboratory management, enabling monitoring of the contents of an explosive precursor cabinet, tracking of the air flow rates of fume hoods, and control of the operation of the canopy hood of an automated chemical synthesis robot. In Figure 5.4, the application interface for monitoring and control of the canopy hood is displayed. The team created and represented three-dimensional models of both the automated chemical synthesis robot and its corresponding canopy hood within the knowledge graph and demonstrated the control of the canopy hood's exhaust air flow rate via the Augmented Reality application. Figure 5.4 (b), (c) and (d) show the user adjusting the exhaust air flow rate of the canopy hood from 1,000 m^3/hr to 900 m^3/hr via the Augmented Reality application, which is reflected in real-time in the laboratory.

The team further developed an Asset Management mobile application to facilitate users to access and interact with assets in the CARES office and laboratory, and to automate repetitive tasks. In the management of a research laboratory, which may span multiple rooms and/or buildings, the ability to access relevant information on the go ensures ease of access and saves time spent browsing through multiple documents. The developed mobile application, working in conjunction with an Asset Management Agent, has three key features: (1) Scanning the asset Quick Response (QR) code to retrieve asset data from the knowledge graph; (2) Instantiating new assets into the knowledge graph; and (3) Printing QR codes. An open-source Identity and Access Management solution (Keycloak) has been deployed within the mobile application to support authorisation and access management services. The authorisation code and access token model implemented by Keycloak are based on the OAuth 2.0 authorisation framework (RFC 6749). This ensures that only authorised users can make changes to the asset information. By utilising this Asset Management mobile application in the CARES laboratory, the time taken to obtain asset information has been reduced from the conventional 2–3 minutes to 5 seconds.

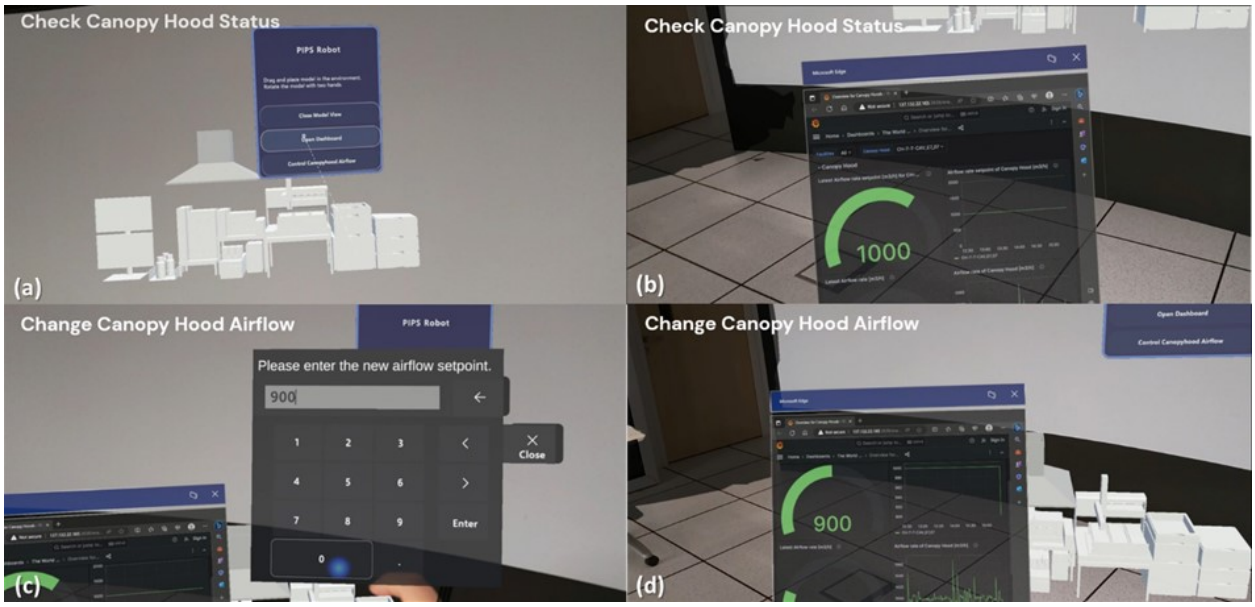


Figure 5.4: Augmented Reality application for the CARES laboratory, illustrating the monitoring and control of the canopy hood of an automated chemical synthesis robot.

Lastly, the team has developed the OntoAsset-Management ontology to represent the assets in the CARES office and laboratory, as well as documents related to the purchase and use of these assets, including purchase requests, invoices, and manuals. The OntoAssetManagement ontology also utilises concepts from various existing ontologies, such as the Purchase-To-Pay Ontology (P2P-O) for purchase document concepts and the Financial Industry Business Ontology (FIBO) for person and organisation concepts. By leveraging the previously developed OntoBIM ontology, instances are linked to their corresponding physical representations in specific rooms or facilities within the building.

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.

Covalency-Aided Electrochemical CO_2 Reduction to CO on Sulfide-Derived Cu–Sb

Daniel Yong Yi Goh, Kah Meng Yam, Lavie Rekhi, Albertus Denny Handoko, Ying Chuan Tan, Yong Wang, Joel Ming Rui Tan, Tej Salil Choksi, Yanwei Lum, and Lydia Helena Wong, *Journal of Materials Chemistry A*

DOI: 10.1039/D3TA04777F

Abstract: p-Block dopants like sulfur have been shown to break scaling relations in the electrocatalytic CO_2 reduction reaction (CO_2RR) by providing alternative binding sites with altered *CO binding energy. However, most sulfide-derived catalysts reported to date tend to produce formate or hydrogen during the CO_2RR by shifting the reaction pathway away from C-bound intermediates. In this work, we discovered highly selective CO production on a bimetallic Cu–Sb–S derived catalyst. The high CO selectivity is in contrast with the individual control samples of CuS_x and SbS_x that demonstrate a preference towards the formate product. Interestingly, different starting phases and atomic ratios of Cu–Sb–S affect the CO_2RR selectivity. Post-catalysis characterization coupled with DFT calculations indicates that the key enabler towards CO formation is the substitution of Sb sites with sulfur which improves *COOH binding relative to *CO, breaking scaling relations and facilitating subsequent CO (g) formation. The highest CO production of FE_{CO} = 80.5% was observed on the tetrahedrite Cu–Sb–S-derived sample at −1.0 V RHE with 37.6 mA cm^{-2} geometric partial current density.

Best practices for oxygen electrocatalysis

Yubo Chen, Daniel Zheng, Jason Zhichuan Xu, and Yang Shao-Horn, *Nature Sustainability*

DOI: 10.1038/s41893-024-01285-y

Abstract: Oxygen electrocatalysis is key for energy conversion and storage technologies such as fuel cells and water electrolysers. However, the measurement of the performance of electrocatalysts is not standardized. This Comment addresses emerging pitfalls in performance evaluation and discusses best practices for oxygen electrocatalysis. With increasing chemical diversity of oxygen electrocatalysts, it has become more challenging to collect reliable electrochemical data and conduct rigorous performance comparisons. Here we outline general considerations for activity evaluation, with specific guidelines for the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER). We then suggest stability evaluation strategies and techniques, and advocate for further performance evaluation using liquid alkaline electrolysers or membrane electrode assemblies (MEAs). In addition, we emphasize that the recommended procedures here might not be universally applicable. For a specific experiment, the best practices should be still considered case by case.

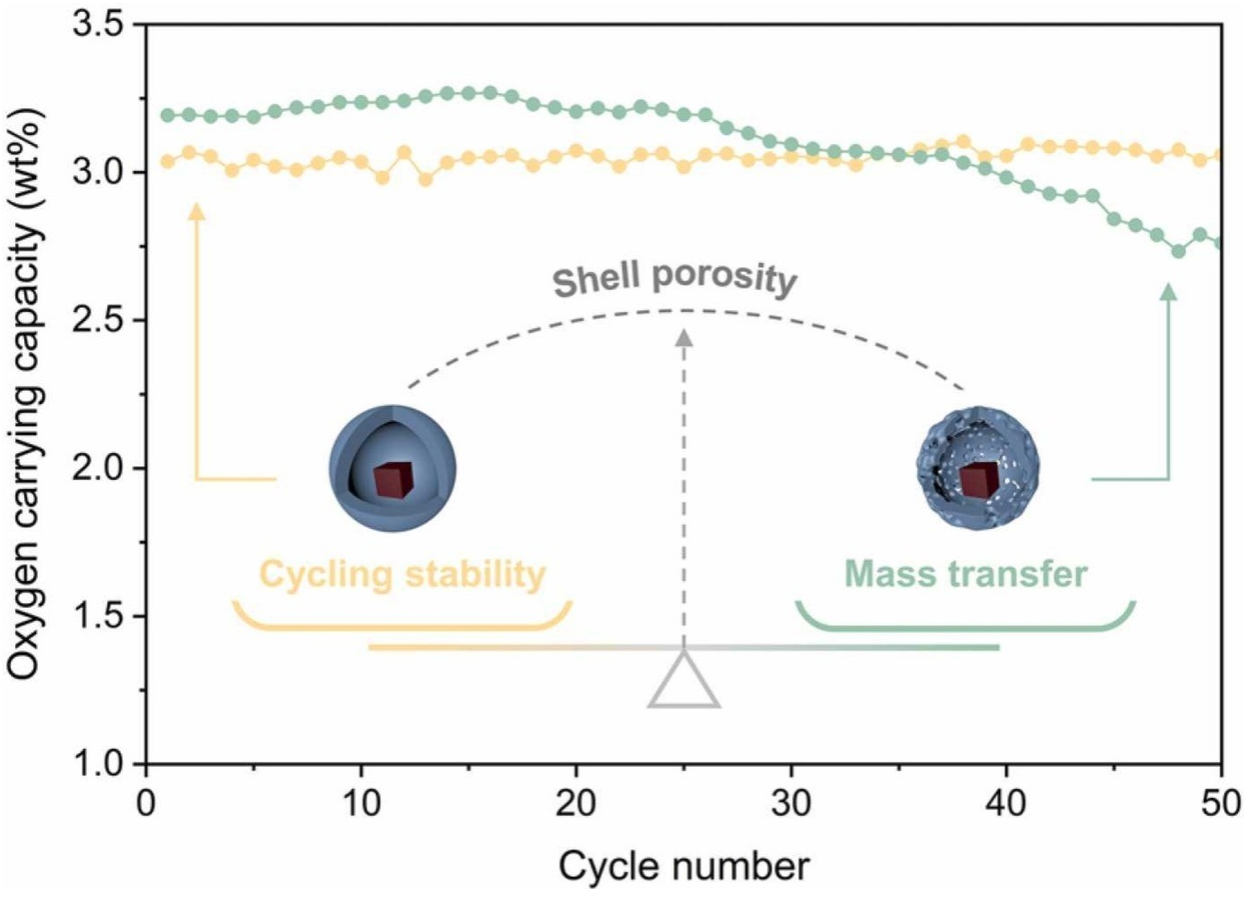
Synthesis of uniform Fe2O3@Y2O3 yolk–shell nanoreactors as chemical looping oxygen carriers

Fan Qianwenhao, Mingwu Tan, Bingqing Yao, Syed Saqline, Longgang Tao, Qian He, and Wen Liu,

Applied Catalysis B: Environment and Energy

DOI: 10.1016/j.apcatb.2024.123935

Abstract: Iron-based materials are extensively employed as oxygen carriers in chemical looping processes, but their long-term performance is often inhibited by sintering and agglomeration. Here, we developed a yolk–shell structured Fe_2O_3@Y_2O_3 oxygen carrier, with each unit consisting of a Y_2O_3 shell encapsulating a nano-sized Fe_2O_3 core. The Y_2O_3 shell could protect the redox -active cores from sintering, and the void between the yolk and the shell is capable of tolerating cyclic volume and phase changes. During the simulated chemical looping cycles at 600 °C, the Fe_2O_3@Y_2O_3 oxygen carriers exhibit a consistent oxygen carrying capacity of 3 wt% over 50 cycles, without any distinguishable structural deterioration. With rational structure optimization, the Fe_2O_3@Y_2O_3 oxygen carriers with porous shell could enhance the mass transfer across the shell and enable higher reaction rates. The satisfactory sintering resistance of the Fe_2O_3@Y_2O_3 nanostructure demonstrates the feasibility of employing well defined yolk–shell structured oxygen carriers for chemical looping applications.

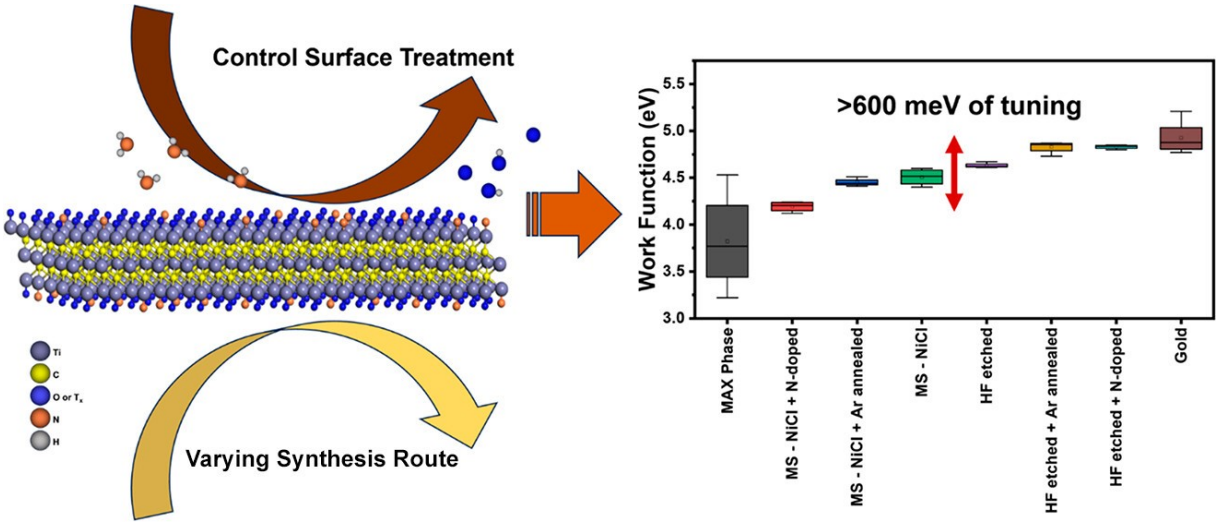


Tuning the Work Function of MXene via Surface Functionalization

See Wee Koh, Lavie Rekhi, Arramel, Muhammad Danang Birowosuto, Quang Thang Trinh, Junyu Ge, Wei Yu, Andrew Wee, Tej Choksi, and Hong Li, *ACS Applied Materials & Interfaces*

DOI: 10.1021/acsami.3c11857

Abstract: MXenes, a class of two-dimensional materials, have garnered significant attention due to their versatile surface chemistry and customizable properties. In this study, we investigate the work function (WF) tuning capabilities of MXene $Ti_3C_2T_x$, where T_x denotes the surface termination, synthesized via both conventional hydrogen fluoride-etched and recently reported molten salt -etched routes. When MXene samples are subjected to gas phase reactions, WF variations exceeding 0.6 eV are achieved, highlighting the potential for precise WF control. Notably, the WF increases from ~4.23 eV (in N-doped MXene etched using molten salt) to ~4.85 eV (N-doped MXene etched using HF). Complementary density functional theory (DFT) calculations reveal WF tuning across a >1 eV range via modification of the surface with different terminal groups (bare metal, F*, O*, N*, and Cl*). These changes in WF are attributed to surface termination modifications and the formation of TiO_2 and TiN phases during annealing. DFT calculations further unveil an inverse correlation between the WF and the electron affinity of surface terminations. The findings from this comprehensive study provide insights into the tunable WF of MXenes, paving the way for their potential applications as interfacial layers in photovoltaic, energy conversion, and storage technologies.



The design and optimization of heterogeneous catalysts using computational methods

Shambhawi, Ojus Mohan, Tej Choksi, and Alexei Lapkin, *Catalysis Science & Technology*

DOI: 10.1039/D3CY01160G Z

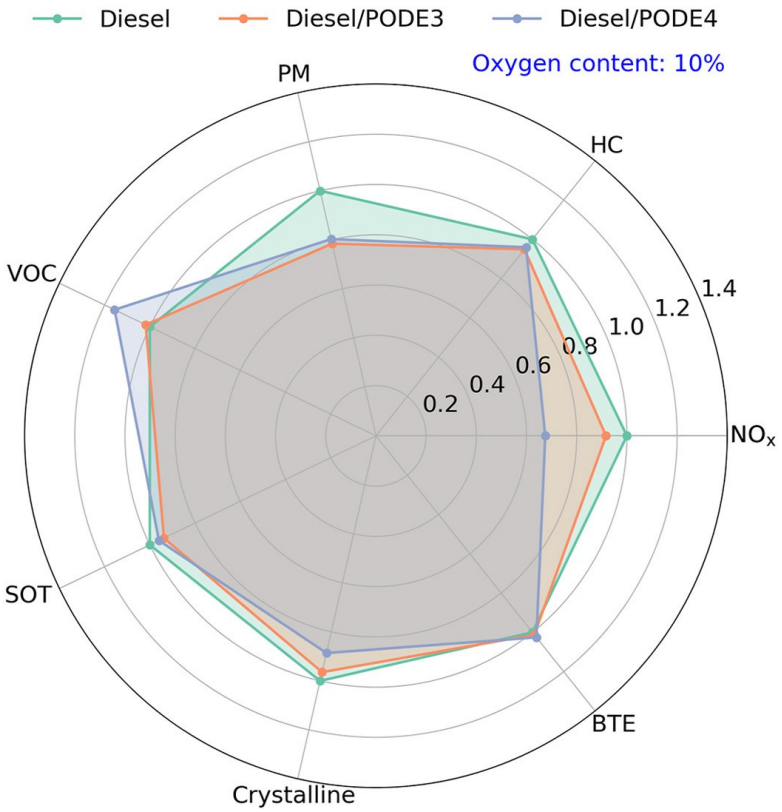
Abstract: The computational design of catalytic materials is a high dimensional structure optimization problem that is limited by the bottleneck of expensive quantum computation tools. Current implementations of first principles computational models for catalyst design are data-hungry, problem-specific and confirmatory in nature. However, they can be made less data-dependent, more transferable and exploratory by developing both forward and inverse catalyst mapping tools that are either inexpensive correlations, like scaling relations, or regression models that are based on relevant descriptors analysis. This work reviews the current application and the possible landscape for future advancements of such tools for developing generalized schemes for catalyst design and optimization.

Comparative analysis of PODE3 and PODE4 fuel additives for emission reduction and soot characteristics in compression ignition engines

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

DOI: 10.1016/j.energy.2023.129498

Abstract: Polyoxymethylene dimethyl ethers (PODEn) have been regarded as promising fuel additives in reducing engine emissions due to their extra oxygen content and absence of C–C bonds. This research compares the effectiveness of PODE3 and PODE4 as fuel additives (10 % oxygen content) in a compression ignition (CI) engine. The results show that PODE can retard the ignition delay and shorten the combustion duration. They can both reduce HC emissions, with PODE4 having the greatest reduction. Both additives comparably reduce NO_x emissions while consuming similar oxygen amounts. PODE alters particle size distribution, favoring higher nucleation mode particles and reducing accumulation mode particles, especially for the case with Diesel/PODE3. Further, this study investigates the soot characteristics when with different fuel blends. Thermogravimetric analysis (TGA) reveals enhanced oxidative reactivity in soot when with Diesel/PODE3 and Diesel/PODE4 fuel blends. Raman spectroscopy shows reduced crystalline structure and increased crystalline width in soot when with PODE additives. Fourier transform infrared (FT-IR) spectroscopy indicates improved relative intensity of aliphatic *C*–H groups and intensified aromatic *C*–H groups with PODE addition. In summary, PODE3 and PODE4 are promising CI engine fuel additives, substantially reducing particulate matter (PM) emissions and enhancing soot reactivity. These findings hold significance for cleaner combustion technologies.



Essential role of lattice oxygen in methanol electrochemical refinery toward formate

Fanxu Meng, Qian Wu, Kamal Elouarzaki, Songzhu Luo, Yuanmiao Sun, Chencheng Dai, Shibo Xi, Yubo Chen, Xinlong Lin, Mingliang Fang, Xin Wang, Daniel Mandler, Jason Zhichuan Xu, *Science Advances*

DOI: 10.1126/sciadv.adh9487

Abstract: Developing technologies based on the concept of methanol electrochemical refinery (e-refinery) is promising for carbon-neutral chemical manufacturing. However, a lack of mechanism understanding and material properties that control the methanol e-refinery catalytic performances hinders the discovery of efficient catalysts. Here, using ^{18}O isotope–labeled catalysts, we find that the oxygen atoms in formate generated during the methanol e-refinery reaction can originate from the catalysts' lattice oxygen and the O-2p-band center levels can serve as an effective descriptor to predict the catalytic performance of the catalysts, namely, the formate production rates and Faradaic efficiencies. Moreover, the identified descriptor is consolidated by additional catalysts and theoretical mechanisms from density functional theory. This work provides direct experimental evidence of lattice oxygen participation and offers an efficient design principle for the methanol e-refinery reaction to formate, which may open up new research directions in understanding and designing electrified conversions of small molecules.

Spin-related Cu-Co pair to increase electrochemical ammonia generation on high-entropy oxides

Shengnan Sun, Chencheng Dai, Peng Zhao, Shibo Xi, Yi Ren, Hui Ru Tan, Poh Chong Lim, Ming Lin, Caozheng Diao, Danwei Zhang, Chao Wu, Anke Yu, Jie Cheng Jackson Koh, Wei Ying Lieu, Debbie Hwee Leng Seng, Libo Sun, Yuke Li, Teck Leong Tan, Jia Zhang, Zhichuan J. Xu and Zhi Wei She, *Nature Communications*

DOI: 10.1038/s41467-023-44587-z

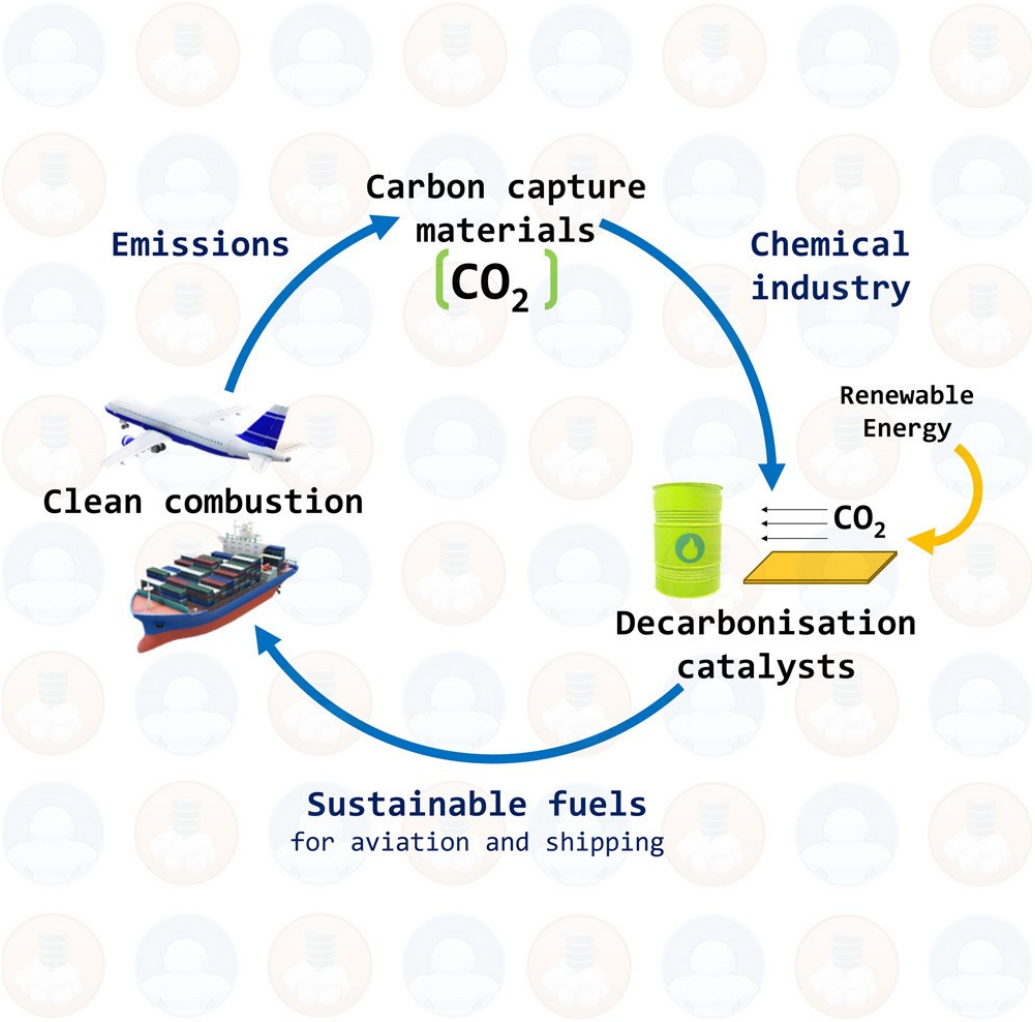
Abstract: The electrochemical conversion of nitrate to ammonia is a way to eliminate nitrate pollutant in water. Cu-Co synergistic effect was found to produce excellent performance in ammonia generation. However, few studies have focused on this effect in high-entropy oxides. Here, we report the spin-related Cu-Co synergistic effect on electrochemical nitrate-to-ammonia conversion using high-entropy oxide $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$. In contrast, the Li-incorporated MgCoNiCuZnO exhibits inferior performance. By correlating the electronic structure, we found that the Co spin states are crucial for the Cu-Co synergistic effect for ammonia generation. The Cu-Co pair with a high spin Co in $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$ can facilitate ammonia generation, while a low spin Co in Li-incorporated MgCoNiCuZnO decreases the Cu-Co synergistic effect on ammonia generation. These findings offer important insights in employing the synergistic effect and spin states inside for selective catalysis. It also indicates the generality of the magnetic effect in ammonia synthesis between electrocatalysis and thermal catalysis.

Hacking decarbonization with a community-operated CreatorSpace

Aleksandar Kondinski, Sebastian Mosbach, Jethro Akroyd, Andrew Breeson, Yong Ren Tan, Simon Rihm, Jiaru Bai, and Markus Kraft, *Chem*

DOI: 10.1016/j.chempr.2023.12.018

Abstract: The pressing challenge of decarbonization encompasses a vast combinatorial space of interlinked technologies, thus necessitating an increased reliance on artificial intelligence (AI)-assisted molecular modeling and data analytics. Our backcasting analysis proposes a future rich in efficient decarbonization technologies, such as sustainable fuels for aviation and shipping, as well as carbon capture and utilization. We then retrace the path to this proposed future with the guidance of two constraints: the maximization of scientists' creative capacities and the evolution of a world-centric AI. Our exploration leads us to the concept of a "CreatorSpace," a distributed digital system resembling existing hackerspaces and makerspaces known for accelerating the prototyping of new technologies worldwide. The CreatorSpace serves as a virtual, semantic platform where chemists, engineers, and materials scientists can freely collaborate, integrating chemical knowledge with cross-scale, cross-technology tools, and operations. This streamlined molecular-to-process-design pathway facilitates a diverse array of solutions for decarbonization and other sustainability technologies.



Other activities and achievements

Sustainable Reaction Engineering

Asst Prof Paul LIU's (PI, NTU) group delivered presentations at the conferences below:

- Oral presentation of "Halite-Structured (MgCoNiMnFe)Ox High Entropy Oxide (HEO) for Chemical Looping Dry Reforming of Methane (CL–DRM)" at the Asian-Pacific Catalysis Congress on 2 November 2023.
- Poster presentation of "CO_2 Hydrogenation to Methanol", "In situ CO2 Capture and Catalytic Hydrogenation ", and "Flame Aerosol Synthesized Copper Based Oxide Catalyst for Electrochemical Reduction of Carbon dioxide" at the CARES 10th Anniversary Scientific Showcase on 1 December 2023.
- Poster presentation of "Halite-Structured (MgCoNiMnFe)Ox High Entropy Oxide (HEO) for Chemical Looping Dry Reforming of Methane (CL–DRM)" at ACS Spring 2024 from 17 – 21 March 2024.
- Oral presentation of "Halite-Structured (MgCoNiMnFe)Ox High Entropy Oxide (HEO) for Chemical Looping Dry Reforming of Methane (CL–DRM)" at ACS Spring 2024 from 17 – 21 March 2024

Asst Prof Tej CHOKSI's (PI, NTU) group attended ACS Spring 2024 from 17 – 21 March in New Orleans, Louisiana. His group activities as below:

- Oral presentation of "A High-Throughput Approach to Determine the Adhesion Energies and Sintering Temperatures of Supported Metal Catalysts."
- Oral presentation of "Designing Low-Dimensional Supported Metal Catalysts for Electrocatalytic Oxygen Reduction by Circumventing Bond Order Conservation-based Scaling Relations."
- Poster presentation of "The mechanism, Kinetics, and role of OH radicals in ultrasound-mediated aqueous glyoxal oxidation."
- Oral presentation of "Tuning the Selectivity for CO_2 Electro-reduction using Electronic Metal Support Interactions: Insights from First Principles Calculations"
- Oral presentation of "Mechanism of ultrasound-driven OH-mediated aqueous benzyl alcohol oxidation with analogies to atmospheric chemistry"

Prof Ning YAN (PI, NUS) was named a 2023 Highly Cited Researcher by Clarivate in the Cross -Field category.

Electrolysis

Dr Chencheng DAI (Research Fellow, NTU) submitted two new technical disclosures:

- A Membrane Electrode Assembly Glycerol Reformer to Suppress Product Crossover and C-C Bond Coupled with Energy-efficient Hydrogen Cogeneration. Other inventors are **Prof Jason Zhichuan XU (PI, NTU)** and **Prof Adrian FISHER (PI, CAM).**
- An ammonia e-cracking cell with alternating electrodes for durable performance. Other inventors are **Dr Tianze WU (Research Fellow, NTU)**, Prof Xu, and Prof Fisher.

One of Dr Dai's previous technical disclosures is being merged with a new submission "Acid-Alkali Membrane Electrode Assembly Electrolyzer For Hydrogen Production By Ammonia E-Cracking" which has been converted to a PCT patent application. Other inventors are Dr Kamal ELOUARZAKI (Co-Founder of Datumelectronix, C4T spin-off), Prof Xu, and Prof Fisher.

Prof Xu is the Lead PI for a new grant "Low-Carbon Energy Research (LCER) Project, Directed Hydrogen Programme (DHP)". The project also involves Prof Fisher.

Prof Xu was named a 2023 Highly Cited Researcher by Clarivate in Chemistry and Materials Science.

Maritime Decarbonisation

The maritime decarbonisation group had a booth and presented scientific posters "Ship-scale emissions dispersion: calculations", "Engine emissions simulations with complex chemistry", "Decarbonising maritime transport - the big picture", and "Decarbonising maritime transport - the detailed options" at the CARES 10th Anniversary Scientific Showcase on 1 December 2023 at Shaw Foundation Alumni House in Singapore.

Dr Li Chin LAW (Research Fellow, CARES) presented "On-board LNG reforming and simultaneous carbon capture: an alternative decarbonization option for the maritime industry" at the 17th Annual Conference of Marine Technology in Athens, Greece from 11-12 November 2023.

Dr Law launched a spin-off company called EMICAST that will offer advanced visualisation of ship emissions through rigorous carbon accounting and forecasting techniques. This service will ensure shipping owners are optimising their operations and cost while meeting regulatory standards. The founding team includes Mr Charalampos SOULTATIS (ADK Maritime), Dr Savvas GKANTONAS (CAM), and **Prof Epaminondas MASTORAKOS (PI, CAM)**. Dr Law had an exhibition booth for EMICAST at the Singapore Shipping Association Tech Show on 22 March 2024.

Dr Law has copyright and docketed the EMI-Ship Sizing model as software (copyright) by NTUitive. This model serves as the foundation for developing new technology/software in the future.

Dr Law and Prof Mastorakos have also signed an NDA with Laskaridis Shipping and METIS Cybertechnology for potential joint research and collaborations.

Dr B HARIKRISHNAN (Research Fellow, CARES) presented "LES-DCMC of dual-fuel ignition problems" at AIAA Scitech 2024 Forum in Orlando, Florida from 8 - 12 January 2024.

Dr Mutian MA (Research Fellow, CARES) has been in discussion with the Maritime & Port Authority of Singapore on the collaboration of ammonia leaking and combustion emission detection using drone and sensors. He has also been in discussion with the Global Centre for Maritime Decarbonisation on the detection of controlled release of ammonia using drone and sensors.

Carbon Policy

Dr J. Lemuel MARTIN (Research Fellow, NTU) presented "Feasibility of Green Hydrogen-Based Synthetic Fuel as a Carbon Utilization Option: An Economic Analysis" at the 6th Meeting of the French-Singaporean Research Network on Renewable Energy (SINERGIE 2023) in Singapore from 6 - 9 November 2023.

Dr Martin also presented "Feasibility of Green Hydrogen-based Synthetic Fuel as a Carbon Utilization Option: Logistics, Pricing, and Economics" at the CARES 10th Anniversary Scientific Showcase on 1 December 2023 at Shaw Foundation Alumni House in Singapore.

Digitalisation

Dr Aleksandar KONDINSKI (Research Fellow, CARES) presented the poster "Knowledge Engineering of Reticular Materials" at two events:

- The Global Young Scientists Summit (GYSS) in Singapore from 8 – 12 January 2024
- CARES 10th Anniversary Scientific Showcase on 1 December 2023 at Shaw Foundation Alumni House in Singapore

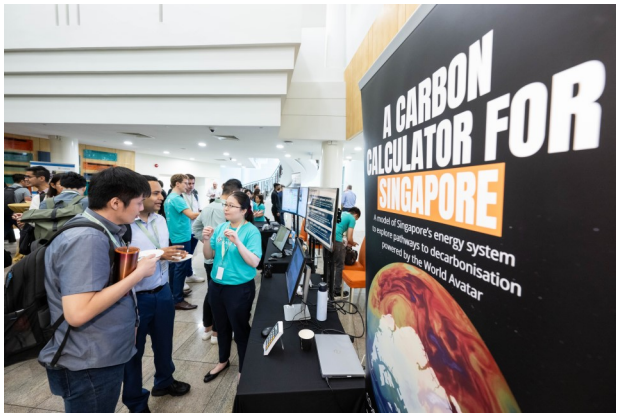
Prof Markus KRAFT's (PI, CAM) group have a paper titled "Question-answering system for combustion kinetics" accepted for presentation at the 40th International Symposium on Combustion in July 2024.

Prof Kraft presented The World Avatar at the following events:

- A knowledge sharing workshop on knowledge graphs and ontologies on 12 October 2023 to A*STAR's Institute for Infocomm Research (I2R).
- KREATIVVITTI is an annual event for the cultural and creative industries launched by Wirtschaftsförderung Pirmasens in Ger-

many. The 2023 edition had the theme "SUSTAINABILITY through creativity & innovation". Prof Kraft gave a talk on 12 November 2023.

- A workshop organised by Arup in Hamburg regarding a digital twin for the city on 15 December 2023. The workshop was regarding applications of knowledge graphs in urban planning, management of public utilities, industrial planning and resilience monitoring illustrated by examples from the group's research in Singapore, as well as applications in Germany and the UK.
- A panellist for ExxonMobil's Technology Conference on the theme "Technology & Future Energy Outlook" on 22 February 2024 in Kuala Lumpur, Malaysia.



Photos from the CARES 10th Anniversary Scientific Showcase:

(top left) Guests in the Auditorium for the Opening Addresses, (top right) Group photo of the CARES programme members, (middle) Guests interacting with the CARES booths, (bottom left) Poster presenters explaining their work.

CLIC

CENTRE FOR LIFELONG LEARNING AND INDIVIDUALISED COGNITION

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

Professor Annabel CHEN Shen-Hsing
Nanyang Technological University

Professor Zoe KOURTZI
University of Cambridge

OVERVIEW

The Centre for Lifelong Learning and Individualised Cognition (CLIC) is a programme within the Science of Learning initiative, harnessing advancements in neuroscience to develop lifelong learning programmes. CLIC is dedicated to enhancing lifelong learning and cognitive adaptability through pioneering interdisciplinary research, with the goal of translating discoveries into a practical model of learning applicable to everyday context.

The study received a six month no-cost extension, which allowed the team the needed time to develop a classroom friendly game for cognitive flexibility from a pilot project, sufficient time to conduct in-depth analysis of the rich dataset acquired during Phase 1, and to produce quality research outputs to journals and conferences in the timeframe. Besides effectively concluding Phase 1 of the study, the extension also accommodates the completion of renovations for the new CLIC office at CREATE tower. We are especially looking forward to physically joining our colleagues at CARES by mid-2024.

The School Workgroup has been progressing well with the adolescents' pilot project, specifically the Bridging Game Project. However, due to the scheduling constraints of the school calendar, data collection had to be pushed to start later than anticipated which caused some delays. The game serves as an ecologically valid assessment tool to gauge cognitive flexibility within a classroom setting. The Bridge Game aims to connect the divide between cognitive science and practical education by offering an authentic means of evaluating students' cognitive flexibility. Currently, the pilot sessions of the project are planned for April to May 2024 and the game is expected to be ready by August 2024.

The extended timeline of Phase 1 of our research also allows for the workgroups to conduct in-depth analyses of the behavioural data as well as the neuroimaging data. Modelling methods were carried out, and an analysis was conducted to understand task performance on various cognitive tests. These analyses inform the cognitive task battery to be used in Phase 2 of the study and will also help in the development, design, and adjustments required for various pilots of the Structure Learning-based Cognitive Flexibility Training Suite (SLiCX).

The Neuroimaging Workgroup is continuing research on protocol optimisation of the pulse sequences, setting up an agreement with the Siemens technical team to implement the sequence and advancing the preparation setup for data acquisition in Phase 2. The team has formulated and tested the data processing and analysis pipeline on a smaller dataset and are currently adapting the scripts for batch processing. Complete data analysis across the entire dataset is expected to be completed by June 2024.

Finally, on 1st December 2023, CARES celebrated their 10th Anniversary in Singapore with a scientific showcase at Shaw Foundation Alumni House, NUS. Researchers from CLIC also joined in on the festivities and participated by having a pre-recorded talk from Prof Trevor Robbins and a showcase of scientific posters and booths to in-

form attendees on our research work. Additionally, the team also gave a sneak peek of our upcoming artbook, highlighting artwork created by children from special needs schools that was submitted during the Brainiverse Experience Art Competition in 2023. The art competition's theme "Neurodiversity: No Brain is the Same" drew 61 artwork submissions from 10 special needs schools in Singapore that concluded with 3 winners. The launch of the highly anticipated artbook is slated for late May 2024.

As we embark on Phase 2 of the project, we look forward to CLIC's continual success and are excited about the road ahead.

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) led the preparation and submission of the CLIC Phase 1 Adult main study manuscript (Tong et al., under review) under the supervision of **Prof Trevor ROBBINS (Senior Scientific Advisor, CAM)**, **Prof Barbara SAHAKIAN (Senior Scientific Advisor, CAM)**, and **Prof Victoria LEONG (Co-Deputy Director, NTU)**. The manuscript aims to broaden the understanding of cognitive flexibility and its relevance to academic attainment and creativity. Dr Tong also contributed to a review paper on cognitive training of cognitive flexibility to *Current Opinion in Behavioral Sciences* led by **Prof Zoe KOURTZI (Co-Director, CAM).**

Dr Xinchen FU (Research Fellow, NTU) contributed to the data analysis and manuscript preparation of the infant exploratory studies. She is responsible for testing sessions, data analysis, and manuscript writing for infant creativity testing, making significant contributions to CLIC's research. Dr Fu and Dr Tong co-led the preparation of a review paper on cognitive flexibility across the lifespan, which has been submitted to *Psychological Medicine* under the guidance of Prof Sahakian and Prof Leong.

As project lead for "Assessing cognitive flexibility and creativity in infants," **Ms Natalie Philyra HOO (Research Assistant, NTU)** oversaw recruitment, scheduling, data management, data analysis, and proposing new task batteries for future phases. Ms Hoo also handles the IRB amendments and incident reports for the team, ensuring project compliance.

Ms Ling Zheng TEO (Research Assistant, NTU) is currently working on examining the relationship between infants' executive functions and creativity. She has recently developed a task battery for infants as young as 12 months to measure their creative potential. Under Prof Leong's guidance, Ms Teo published the creativity task battery, including Music Play, Object Play, and Exploratory Play, which examines infants' creative potential in the journal *MethodsX*.

The Cognition Workgroup showcased the CLIC research at the CARES 10th Anniversary Scientific Showcase on 1 December 2023 at Shaw Foundation Alumni House in Singapore. Ms Hoo contributed to designing the infant study poster and presented the methodology and brief findings to attendees. Dr Fu and Dr Tong presented CLIC's research on cognitive flexibility and creativity in infants and adults to professionals and the public attending the event.

Figure 6.1: Ms. Hoo (1st from left) and Dr Fu (2nd from left) presenting CLIC's research at the CARES 10th Anniversary event.

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 consisting of **Dr Chew Lee TEO (Co-PI, NTU), Dr Peter SEOW (Co-PI, NTU), Dr Nastassja LOPES FISCHER (Research Fellow, NTU), Ms Phillis FU (Research Associate, NTU), Ms Shilpi TRIPATHI (Research Associate, NTU),** and **Ms Gabrielle ONG (Research Assistant, NTU)** have been working on developing a bridge game since October. The game is an ecologically valid measure of cognitive flexibility that can be conducted in the classroom. Unlike traditional lab-based measures of cognitive flexibility, the bridge game attempts to connect the gap between cognitive science and the classroom by providing an authentic way of measuring cognitive flexibility in students. The game involves students designing a bridge using different materials across different dimensions (width and load) and difficulty levels. Students would have to be cognitively flexible in utilising different materials (within a given budget) to build a cost-efficient and effective bridge. Depending on the situational demands, students are tested on their cognitive flexibility in how they adapt to different situations and switch strategies accordingly. Through this game, the team hopes to capture and demonstrate students' cognitive flexibility in a problem-solving context.

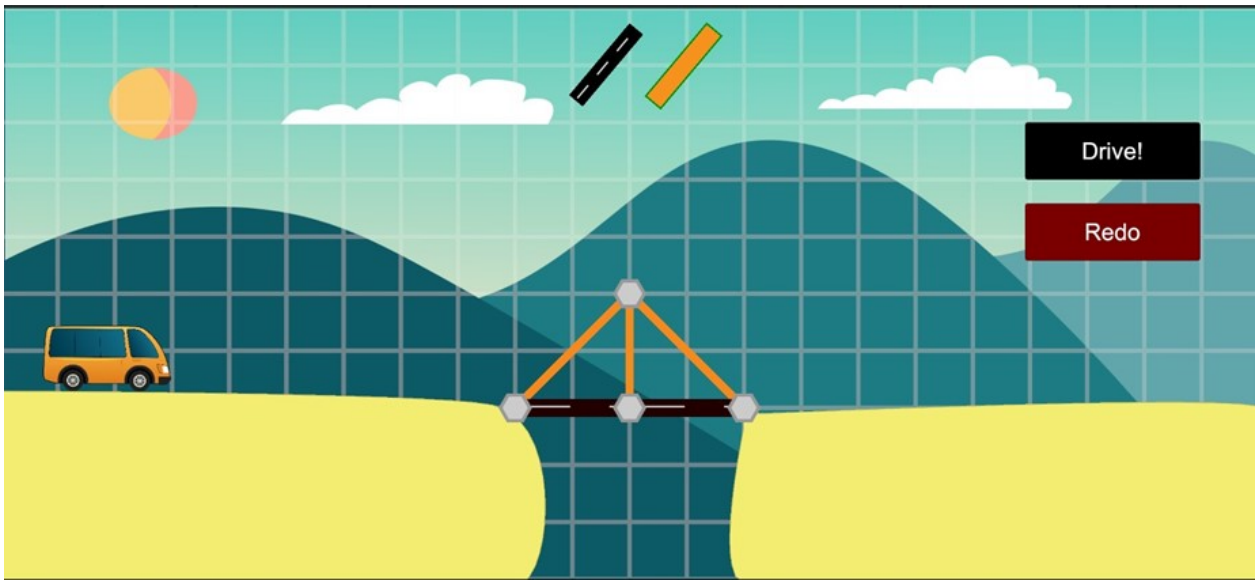


Figure 6.2: Bridge Game interface.

Ms Ong is writing up a grant proposal to fine-tune the bridge game design as well as other pedagogically viable cognitive tasks. This will be done through examining whether the cognitive flexibility of students is improved using the bridge game while learning using pedagogies like Knowledge Building and tinkering.

Ms Fu is collaborating with the Neuroimaging team on the design of the Structure Learning-based Cognitive Flexibility Training Suite (SLiCX). SLiCX intends to use the Structure Learning paradigm to train cognitive flexibility in adolescents and young adults. Bringing her experience in working with adolescents and the design of the Bridge Game, Phillis is working with the Neuroimaging team on the gamification of SLiCX to tackle the motivation issues and to integrate a backstory.

The team is currently validating the Contextual Linguistic Profile Questionnaire (CLiP-Q) among Singaporean adolescents. The paper, provisionally titled "Exploring Language Diversity among

Singapore Adolescents: Psychometric Validation Properties and Confirmatory Factor Analysis of the CLiP-Q Scale", aims to understand and measure language diversity in Singapore's multilingual landscape. This allows for a comprehensive framework for understanding linguistic diversity among adolescents in Singapore, emphasising the importance of a multifaceted approach to linguistic experiences and underscores the need for ongoing exploration in the dynamically evolving linguistic landscape, particularly in light of Singapore's emphasis on bilingualism and multiculturalism.

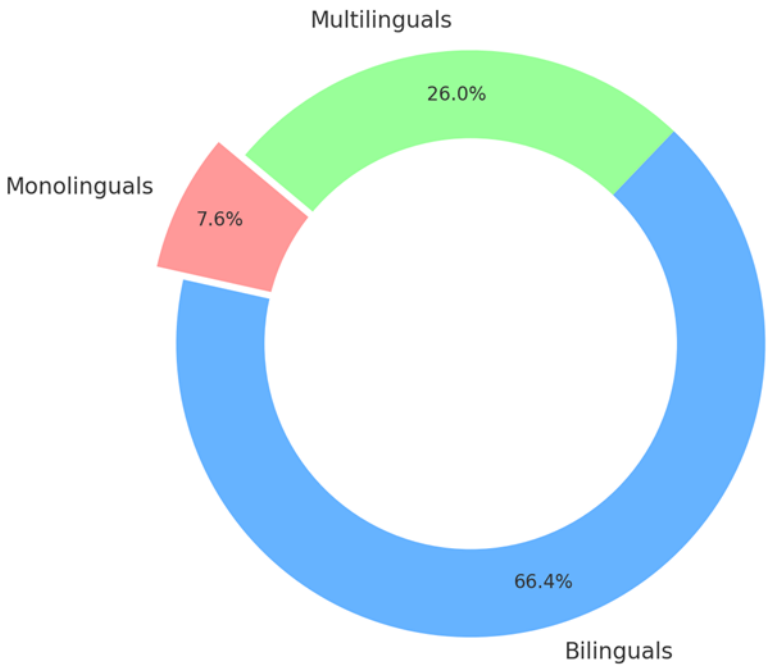


Figure 6.3: Demographic breakdown of adolescent participants by linguistic diversity (N = 347).

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 team is particularly focused on the constructs pertaining to multilingualism, tolerance of uncertainty, perceived social support, social decision-making, and career development. The team has been preparing manuscripts for publication pertaining to 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, CAM) has contributed to the most recent paper by Tong et al. on the Cognitive Flexibility construct, which was recently submitted to *Psychological Science*. She is also advising **Dr Shengchuang FENG (Research Fellow, NTU)** on his paper which uses language entropy as a measure. Prof Hendriks has also been involved with meetings with the School team on the social data geared towards writing up some of the WP0 findings. With regards to the social work package of Phase 2, she has been discussing possible linguistic measures to be added to the larger study. Prof Hendriks is closely involved with the digital artbook produced from the very successful CLIC public outreach events (The Brainiverse Experience) in August and September 2023. A launch for the artbook is also planned to take place in May 2024 with attendance from some of the student artists from special needs schools.

Dr Feng has been working on two manuscripts: (1) "The relationship between language entropy and cooperativeness" and (2) "A database of responses to behavioral game theory tasks in Singapore: A Qualtrics Implementation." (Feng et al., in preparation) In the preparation of the latter manuscript, he has also created a GitHub repository (https://github.com/ntu-cam-clic/Social_Decision_Making_Tasks) to share the scripts and stimuli of the social decision-making tasks. Additionally, he has identified a problematic item in the 10-item short version of the Big-5 Inventory by analysing WP 0.1 and WP 0.2 data, as well as multiple open-source datasets. Currently, he is working on a manuscript focusing on the analysis of this item. Furthermore, he is preparing to demonstrate hands-on analysis of fMRI data at a Professional Development Workshop during the 84th Annual Meeting of the Academy of Management, which will be held on August 2024 in Chicago, USA.

Dr Melia has been preparing manuscripts together with Prof Hendriks for a publication related to social factors, particularly multilingualism. She is currently working on three manuscripts: 1) "Validation of the CILD-Q for Measuring Multilingualism in Singapore", 2) "The Relationship between Multilingualism and Perceived Social Support", and 3) "Multilingualism and Cognitive Flexibility". She is also preparing to present posters for manuscripts (1) and (2) at the 2024 American Psychological Association conference which will be held on August 2024 in Seattle, USA. Dr Melia is also part of the organising committee of the Brainiverse artbook launch to be held in May 2024.

Ms Emma Sam Yoke LOO (PhD Student - IGP-CRADLE) was involved in the logistical and administrative planning for WP0.1, including preregistration, participant recruitment, and data analyses. Additionally, she was also responsible for the cognitive flexibility and career transition/adaptation sub-studies within WP0.1. Her resulting paper on a parsimonious model of Savickas & Porfeli's Career Construction Model of Adaptation was recently accepted for presentation at the April 2024 Asian Management Research Consortium in Singapore.

Mr Akshay ABRAHAM (Research Associate, NTU), **Ms Hui Shan YAP (Research Assistant, NTU)** and **Ms Yuan Ni CHAN (Research Assistant, NTU)** have contributed to the general logistical and administrative planning for studies of the WP0 package (WP0.1). Mr Abraham and Ms

Yap have also conducted a comprehensive literature search into personality scales based on the Big Five personality traits to support future publications, while Ms Chan is working on the analysis of the tolerance of uncertainty as well as the social decision-making data collected from the WP0.1 study.

Ms Megan OH (Research Assistant, NTU) joined CLIC's Social Team in October 2023. She assists with data processing, cleaning, and analysis of the WP0.1 study datasets. Currently, she is conducting data analysis looking at possible factors influencing sleep quality, housing environment, and stress.

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 led by **Dr Eleanor KOO (Research Fellow, NTU)** is collaborating with the other workgroups to plan the Phase 2 Structure Learning (SL) training design as part of SLiCX. The second dimension to be introduced are shapes surrounding the existing symbols, instead of colour (as mentioned in the previous Biannual Report), as a result of discussions and agreements with PIs from all workgroups. Three pilot studies will be rolled out consecutively to test saliency of the new dimension, progression criteria and number of sessions to set for the main study, as well as whether participants are able to identify the dimension of interest without explicit instructions. **Mr Wei Ler KOO (Research Assistant, NTU)** is working on the MATLAB scripts, with the help of **Dr Shengchuang FENG (Research Fellow, NTU)** from the Social team, to implement the new contingencies and stimuli. **Ms Janet TAN (Research Assistant, NTU)** and **Ms Marisha Barth UBRANI (Research Assistant, NTU)** are working with **Ms Phillis FU (Research Associate, NTU)** from the School team to design a cover story for the training to be engaging. Currently, informed consent forms and other necessary IRB amendments have been made and submitted by Ms Ubrani. The SLiCX pilot is scheduled to commence recruitment and data collection in April 2024 pending IRB approval.

Several in depth analyses were conducted on the intervention data in WP0.2:

1. Ms Tan led an analysis to examine the relationships between Structure Learning and inverse temperature, a measure of matching (explore) – maximizing (exploit) dimension of two cognitive flexibility tasks, Intra-Extradimensional task (IED) and Probabilistic Reversal Learning (PRL), with higher values interpreted as greater exploitation tendencies. A regression analysis of inverse temperature of IED and PRL against mean strategy index of SL (for both Stage 1 (easier) and 2 training (more difficult)) found inverse temperature of IED and PRL to have a statistically significant positive relationship with only the mean strategy index of Stage 1 training (Figure 6.4). This suggests that higher inclination to use maximising strategy in SL predicts greater exploitation tendencies in IED and PRL, and that participants carry their strategy tendencies from training to post-training, indicating a learning effect.
2. Ms Tan also examined the relationships between SL variables, such as relative Performance Index (PI) change and mean Integral Curve Difference (ICD), with other cognitive variables. Relative PI change is an indicator of performance change throughout SL and mean ICD is the strategy index used to classify participants' strategy into matching, mixed and maximising.

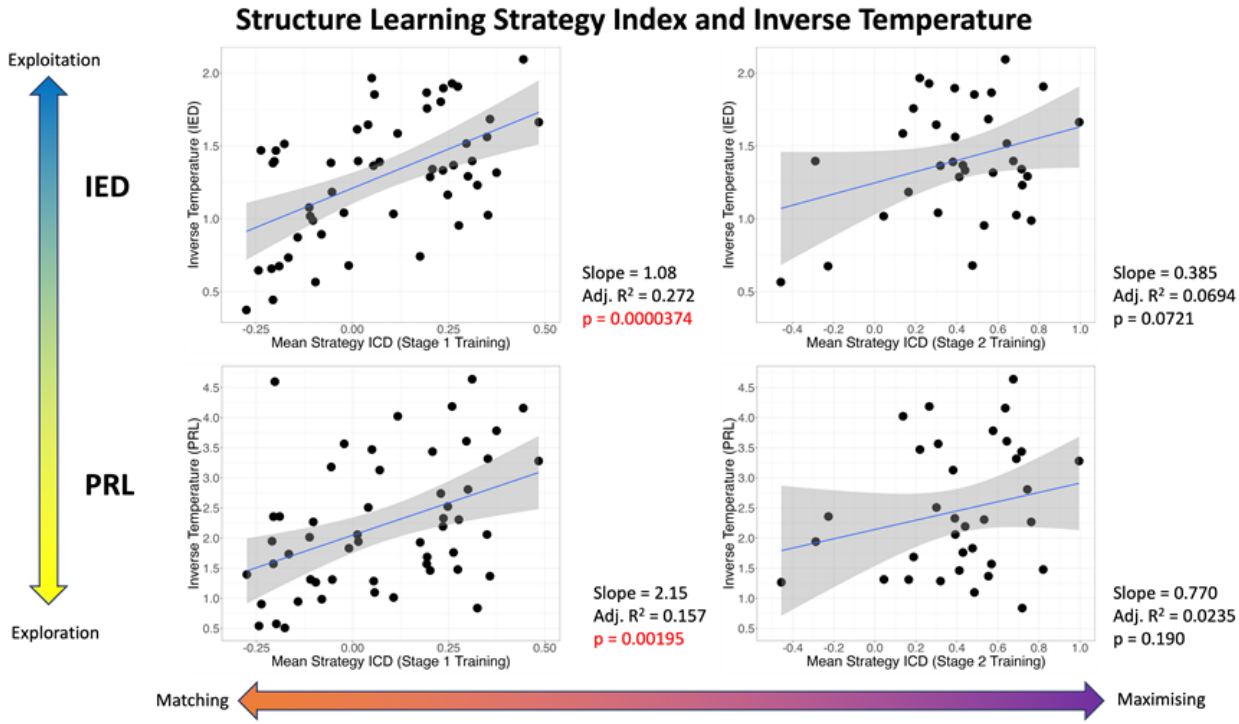


Figure 6.4: Regression plots of inverse temperature of IED and PRL against Mean strategy index of Structure Learning.

A moderate positive relationship between relative PI change and ICD change (r=0.679, p=2.25x10^{-8}) was observed, indicating that switching strategy to a more maximising one improves performance of participants during SL. This corroborates with the team's inspection of individual subject plots, where participants classified as using maximising strategy perform better in the SL training. Higher performance in SL also correlates significantly with better performance of the Task Set Switching Where version (TSS Where) task (r=0.281, p=0.0413). However, the same relationship was not found between relative PI change and other cognitive flexibility tasks. The correlation tests of mean ICD indicated positive relationships with intelligence tasks - Raven's Advanced Progressive Matrices (r= 0.317, p = 0.0207), Wechsler Abbreviated Scale of Intelligence (WASI) Block Design (r= 0.310, p = 0.0241) and WASI Vocabulary (r=0.316, p = 0.0210). Intelligence tasks were administered pre-training; hence this finding supported intelligence to be associated with choice of strategies in SL.

3. Ms Ubrani conducted Bayesian Modelling analysis to examine cognitive flexibility in the Colour Shape Task (CST) pre and post SL training. This analysis compared accuracy (ACC) and reaction time (RT) in shift and repeat trials between control and training groups, following Ye and Damian's [1] methodology. The analysis was used to inspect the raw data more closely as previous analyses relied on formula-derived values such as switch cost (difference between shift and repeat trials). A Bayes Factor (BF) was utilised to provide a hypothesis-testing approach, given that previous analyses suggested performance in both groups could be attributed to the practice effect. Results from Mixed ANOVA with Bayesian Factors showed no main effect of group in ACC or RT. Practice effects were evident, with an increase in response speed over time, $F(1, 106) = 58.97$, $p<.001$, $BF >100$. Notably, an interaction effect, $F(1, 106) = 60.48$, $p<.001$, $BF >100$, was found between trial type (shift and repeat) and the task (shape or color) of the previous trial (n-1) on RT (Figure 6.5). Post-hoc analysis revealed quicker responses when par-

ticipants repeated the color task (M = 783, SD = 23.6) rather than the shape task (M = 801, SD = 25). However, if participants needed to shift tasks, they shifted quicker after shape (M = 927, SD = 29.5) than color blocks (M = 972, SD = 28.8). This highlights the varying responsiveness to different tasks in set-shifting tasks like CST.

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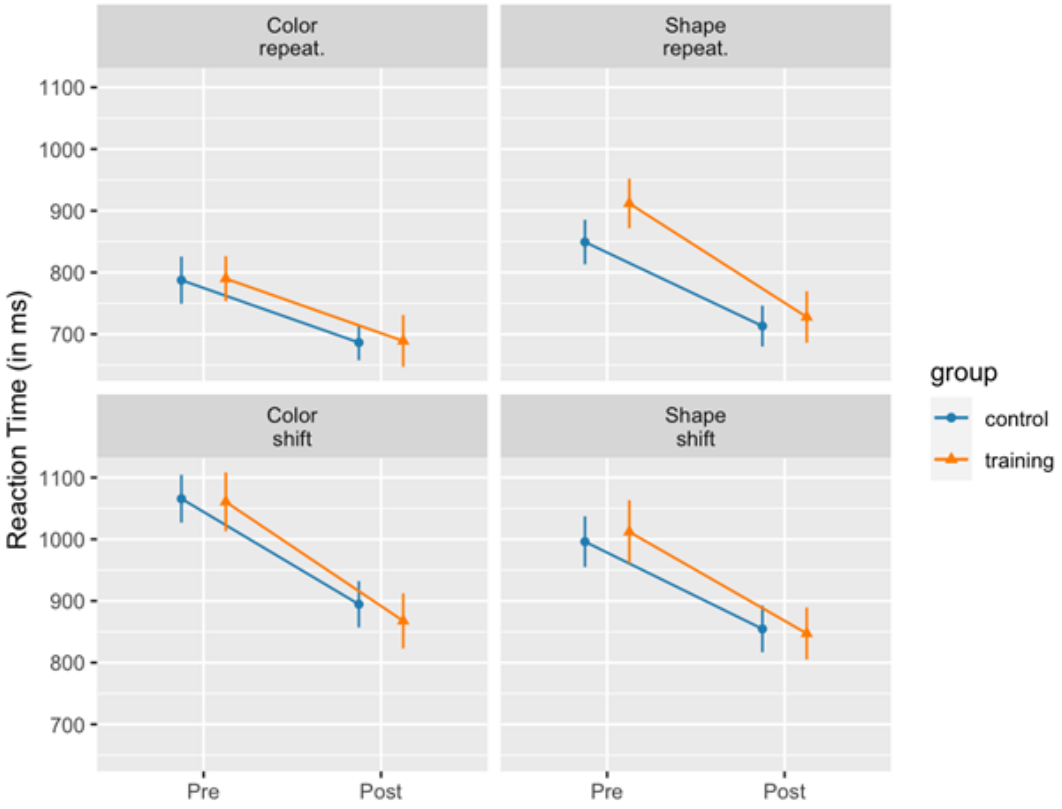
[1] Ye, W., & Damian, M. F. (2022). Exploring task switch costs in a color-shape decision task via a mouse tracking paradigm. *Journal of Experimental Psychology: Human Perception and Performance*, *48* (1), 8-.

[2] Lee, M. D., & Wagenmakers, E. J. (2013). Bayesian cognitive modelling: A practical course. *Cambridge University Press*. https://doi.org/10.1017/CBO9781139087759



F (1, 106) = 60.48, p = <.001
Interaction BF_{10} = 9590

Bayes Factor	Interpretation
>100	"Extreme" evidence for Alternative Hypothesis (H_1)
30 – 100	"Very strong" evidence H_1
10 – 30	"Strong" evidence H_1
3 – 10	"Moderate" evidence H_1
1 – 3	"Anecdotal" evidence H_1
1/3 – 1	"Anecdotal" evidence for Null Hypothesis (H_0)
1/10 – 1/3	"Moderate" evidence H_0
1/30 – 10	"Strong" evidence H_0
1/100 – 1/30	"Very strong" evidence H_0
<1/100	"Extreme" evidence for H_0

Figure 6.5: (Top) Line plots with error bars of RT on the type of trial in the current trial and the task of the previous trial across time points. (Left) Bayes Factor (BF) interpretation employed [2].

Dr Deepika SHUKLA (Research Fellow, NTU) led the neuroimaging analyses for MRS and MPM. A data quality check found some apparent misalignment between original bilateral DLPFCs ROIs placement and the observed ROIs in data processing steps for the MRS data. This took a considerable time to troubleshoot. Nevertheless, the team has managed to resolve the issue and completed the data processing. Figure 6.6 illustrates the consistency of ROI placement, and the data quality achieved in the study between pre- and post-training imaging sessions.

The initial MRS data findings showed a significant reduction in R-DLPFC Glx (p = 0.007, mean-diff: -2.479) compared to control-group (Figure 6.7a). Paired comparison between sessions showed significant decrease in post-training R-DLPFC GABA+ in Training-group (p = 0.03, mean-diff: 0.656) but not in C-group (p= 0.12) (Figure 6.7d), while no significant difference was observed for L-DLPFC GABA+, Glx and GABA+/Glx ratio across groups and sessions. A conference abstract (Neurochemical Alterations in Bilateral DLPFC after Structure Learning Training in Healthy Adults) on the findings will be presented in the upcoming Organisation for Human Brain Mapping 2024 annual meeting from 23 – 27 June in Seoul, Korea. The team is extending the MRS data analysis with behavioural outcomes and preparing a manuscript tentatively entitled "Effect of Structure Learning Training on the Bilateral DLPFC Neurotransmitters and associated Cognitive Flexibility Measures among Healthy Young Adults" with submission targeted for July 2024.

To rectify the extended scan time requirement for manual shimming in the MRS experiments, the team has worked on protocol optimisation and identified the requirement of automated data shimming for MRS acquisitions using advanced sequence FAST (est)MAP for better data quality control. The team is in discussion with the Siemens technical team and CMRR sequence sources to set up C2P agreement to deploy the sequence and preparation setup for data acquisition in Phase 2.

In addition, the team has made progress with the MPM data processing & analysis pipeline design, tested on a small dataset (Figure 6.8). The scripts are being modified for batch processing and complete data analysis is targeted for May 2024.

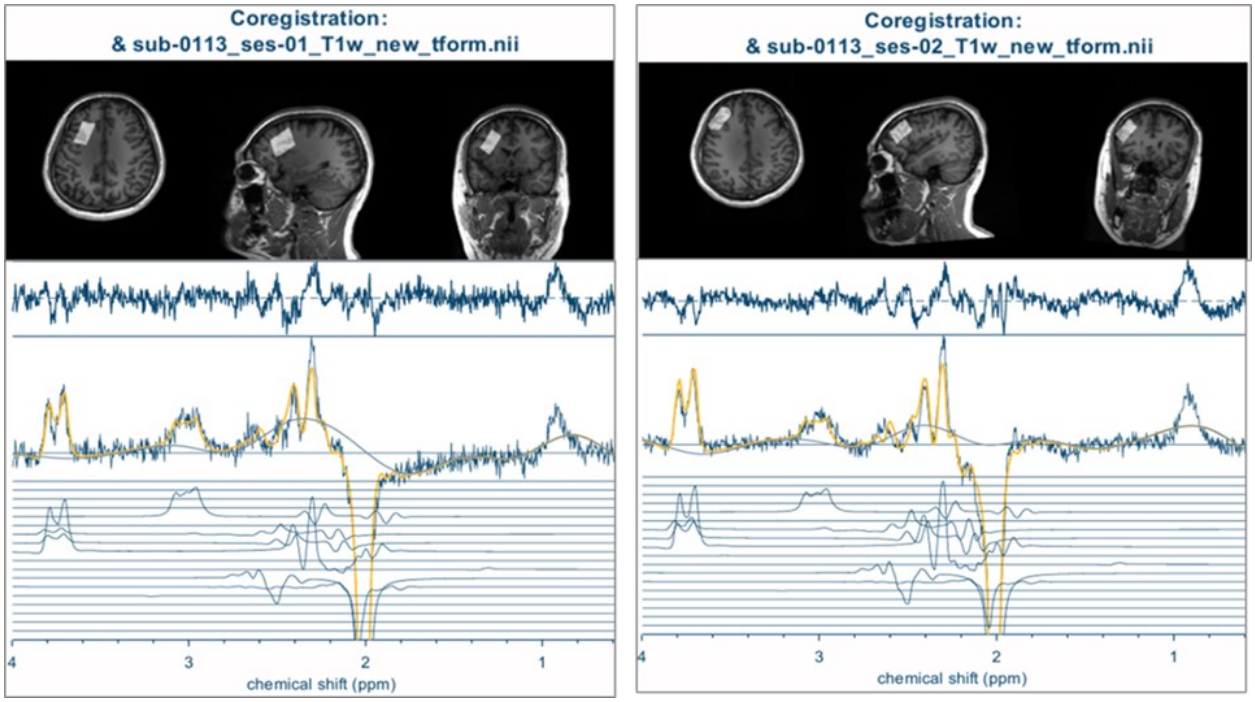


Figure 6.6: ROI placement on left-DLPFC in pre- (ses-01) and post-(ses-02) sessions, along with fitted GABA+ and Glx peaks in the MRS data using Osprey software.

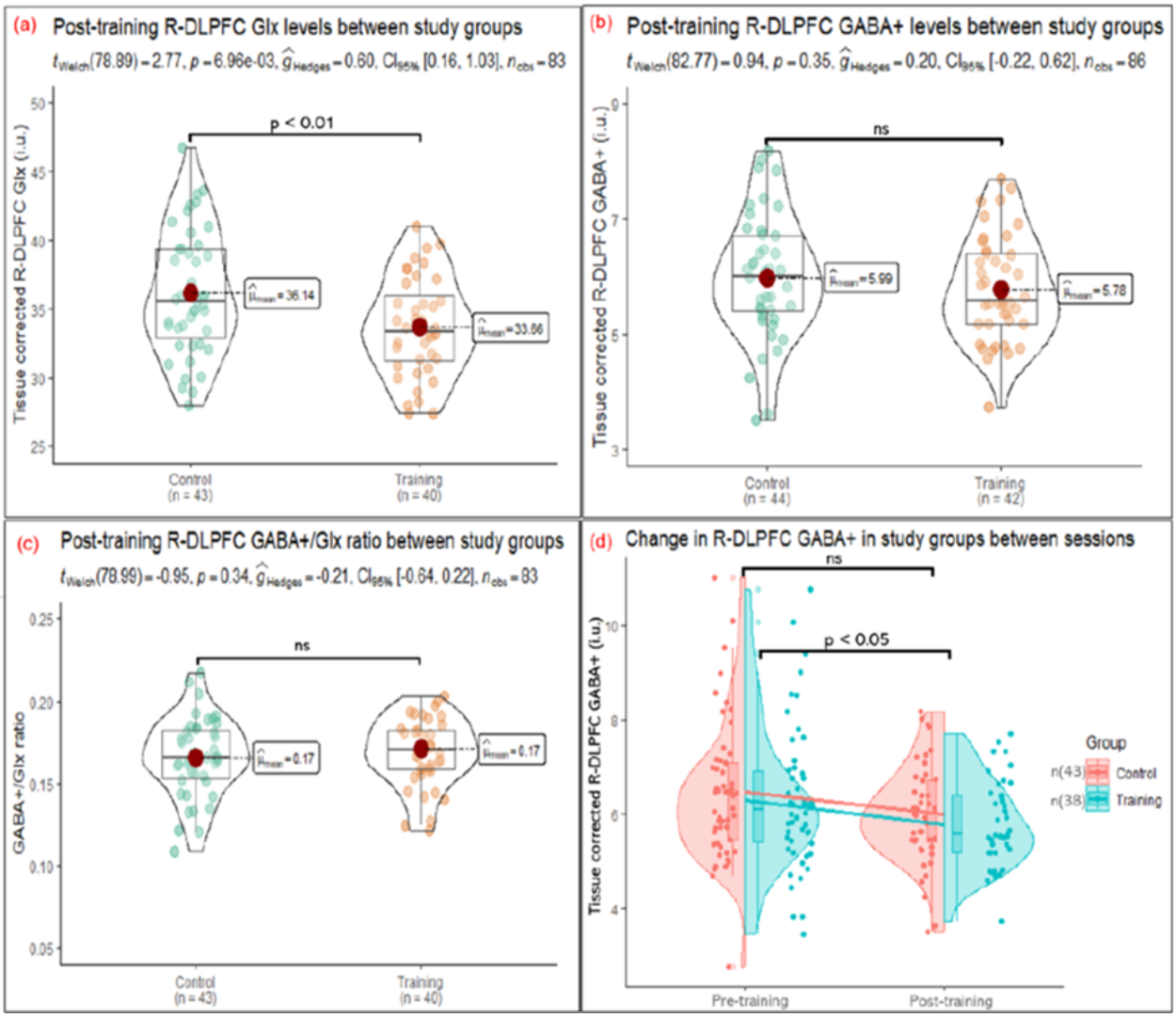


Figure 6.7: Neurochemical alterations in the Left (L)- DLPFC and right (R)-DLPFC between study groups and sessions.

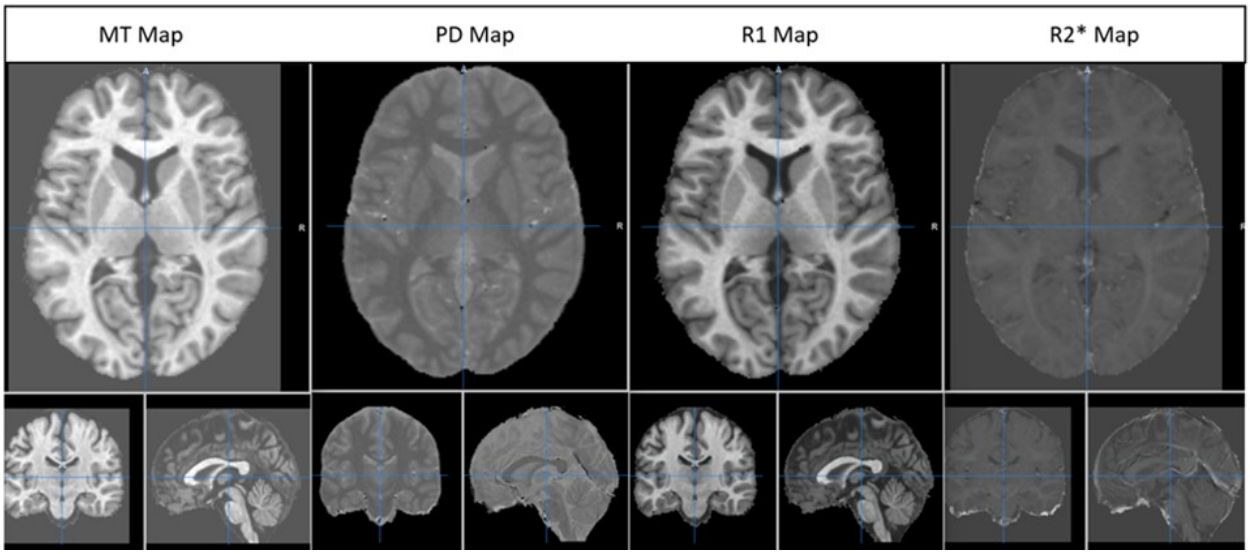


Figure 6.8: An illustrative example of CLIC WP0.2 MPM data and processed Maps generated for further ROI- and group-based data analysis.

Ms Winlynn CHOO (Research Associate, NTU) has been maintaining the CLIC REDCap infratructure (Figure 6.9). The CLIC REDCap servers are composed of UAT and production servers, where the UAT is only accessible via the NTU network and acts as a testing platform for agendas related to REDCap. The production web server is accessible via the internet and is targeted to host the recruitment and survey for Phase 2 of CLIC. Dr Shukla, **Ms Natalie Philyra HOO (Research Assistant, NTU)**, **Ms Shilpi TRIPATHI (Research Associate, NTU)**, and **Ms Yuan Ni CHAN (Research Assistant, NTU)** have been elected as the secondary administrators to help with the roll out of REDCap in Phase 2. They will work alongside Ms Choo to set up questionnaires and decide on member's roles once the surveys for Phase 2 are confirmed. At current stage, there are 2 active trial projects built in REDCap: SLiCX Pilot 1 for CLIC and BrainNorm for CRADLE. Ms Choo also works with Dr Koo and Ms Ubrani to ensure that the details of the DMP provided are accurate.

In preparation for the Phase 2 data analysis, CLIC is working with the NTU High Performance Computing Centre (HPCC) to onboard CLIC servers to NTU HPCC located at NTU North Academic Complex, NS4-02-21. The initiative is led by **Dr Sheng Hung CHUNG (Research Engineer, NTU)** and HPCC team to support the needs of the large-scale data computation for CLIC researchers in Phase 2. The CLIC servers' migration was carried out in April 2024 and High-Performance Services are provided including (i) cluster and nodes integration, (ii) OS tuning and optimisation, (iii) data piping integration and management to support computational-intensive workload. The setup of CLIC servers hosting in NTU HPCC enhanced system security (NTU Security Compliance Policy). NTU HPCC enables only authorised CLIC users listed in NTU AD and strengthens its security by implementing an additional layer of Two-Factor Authentication.

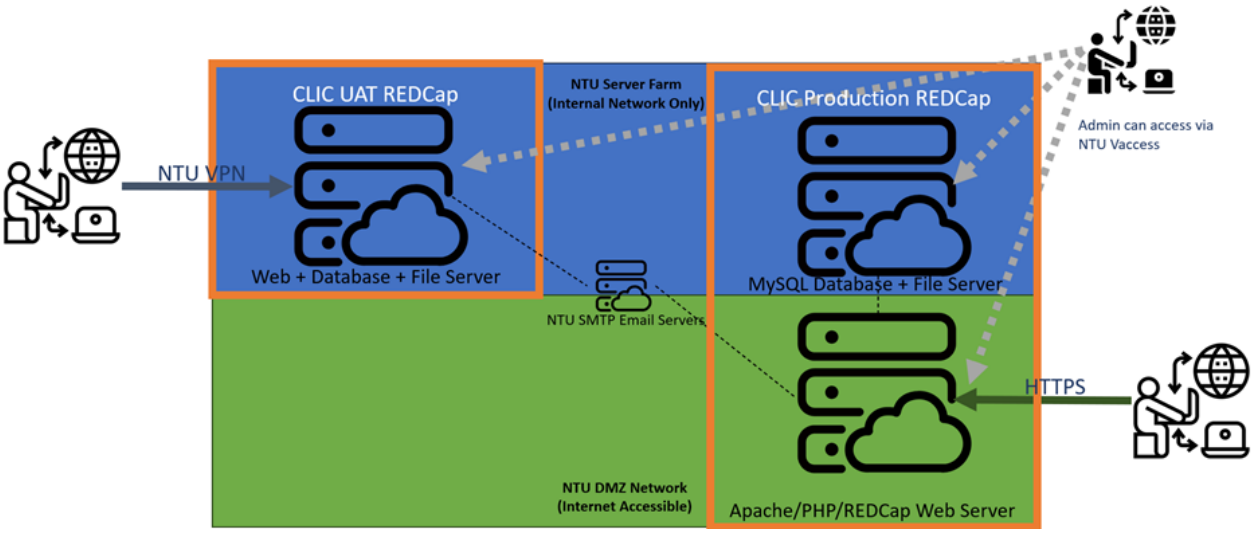


Figure 6.9: CLIC REDCap Infrastructure.

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

Other activities and achievements

Prof Henriëtte HENDRIKS (Co- Deputy Director, CAM) presented "Multilingualism and its relation to executive functions and psycho-social factors: A study of a very multilingual society" on the topic of CLIC and their initial findings at the CNRS, Laboratoire Structures Formelles du Langage on 29 January 2024 in Paris, France.

Dr Deepika SHUKLA (Research Fellow, NTU) and **Dr Eleanor KOO (Research Fellow, NTU)** organised an fMRI workshop for CRADLE and CLIC researchers at NTU on 18, 20, and 21 March 2024. Dr Shukla introduced the basics of fMRI on the first day while Dr Koo conducted the hands-on workshop on fMRI pre-processing, quality check, and analyses on the second and third day. **Dr Sheng Hung CHUNG (Research Engineer, NTU)** presented a briefing on the CLIC servers on the second day.

The School team is collaborating with the Singapore Examination and Assessment Board (SEAB) to develop a measurement for critical, adaptive and inventive thinking skills (CAIT). This collaboration is led by **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)** and supported by **Ms Phillis FU (Research Associate, NTU)** and **Ms Gabrielle ONG (Research Assistant, NTU)**. Through this project, the team will engage with different schools in Singapore that will undergo the assessments for CAIT, cognitive flexibility and creativity. This collaboration provides us an opportunity to create a meaningful impact to education in Singapore and investigate the role of cognitive flexibility and its relationship to classroom learning. The pilot was conducted by SEAB on their CAIT measurement, and the first round of data collection is expected to start in May 2024.

Assoc Prof Georgios CHRISTOPOULOS (PI, NTU) recently received the Leadership, Management and Organization Division Research Award from Nanyang Business School. He delivered invited presentations at the Macau University Business School, Nottingham University (Malaysia Campus), and the 4th Macau Symposium on Cognitive and Brain Sciences from 8-9 September 2023 in Macau SAR, China.

Assoc Prof Christopoulos and **Dr. Nadhilla Velda MELIA (Research Fellow, NTU)** also curated and presented their research on an episode of "NUDGES", a local 5-part documentary series produced by Channel News Asia uncovering the invisible forces behind our choices through the lens of some of our most long drawn struggles.

The episode the team participated in "Snack On Junk Food Often? The Secret To Healthy Eating May Lie In Tricking Your Brain | Nudge" was aimed at educating the public about social decision-making and nudges to eat healthier. The episode has already garnered 323k views (data as of 20 May 2024) on YouTube.

CLIC had a booth and presented scientific posters at the CARES 10th Anniversary Scientific Showcase on 1 December 2023 at Shaw Foundation Alumni House in Singapore. The team also used the event to provide a sneak peek of an upcoming artbook showcasing artwork by student artists from special needs schools that was submitted during the Brainiverse Experience Art Competition in 2023. The theme was "Neurodiversity: No Brain is the Same". The launch of the artbook is slated for late May 2024.

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

OVERVIEW

The AMPLE project – an Accelerated Manufacturing Platform for Engineered Nanomaterials – is developing a next generation nanomaterial synthesis pipeline for high precision and economical 1 to 100 kilograms per day production, using nanoparticle ZnO as a case study. The key goals for the AMPLE project are to construct the 100 kg/day pilot system in CARES' lab, validate the technology in an industrial setting (TRL7-8), develop a plan for commercialisation and raise funds for a successful commercial spin-off. AMPLE's team, a diverse mix of industry professionals with backgrounds from nanomaterials synthesis to microbiology and entrepreneurship, is led by Dr Nicholas Jose and Prof Alexei Lapkin.

To date, AMPLE has constructed three automated systems for synthesis – the K1, K10 and K100 – for 1 to 100 kilogram synthesis, and has demonstrated synthesis capabilities on all systems. Nano zinc oxide products for coatings and cosmetics have been created and formulated in collaboration with both local SME's and MNC's to their requirements, leading to strategic collaborative agreements and future commercial sales. Strategic agreements with multinational distributors for scaling AMPLE's commercialisation efforts have also been created with partners like Kowa Co. Ltd. As AMPLE finishes at the end of Nov 2024, the team aims to undertake factory trials of the K100 technology, patent and productise the IP developed within AMPLE, and prepare the team for a clean transition into Accelerated Materials.

Dr Nicholas Jose, Project Lead

Since our last update in September 2023, AMPLE has had incredible progress, resulting in key technical and commercial developments. The team has also undergone changes, as our Quality Control Scientist (Ms Kencha Umamaheswari) and Automation Engineer (Ms Faye Ng) departed, with Application Chemist Dr Maxim Kiryukhin and Research Assistant Karim Ben Hicham joining.

As mentioned in our last progress report, AMPLE is developing unique, structured nano zinc oxide materials with high performance in coatings. We have successfully scaled to the multi-kilo per day scale with our K10 reactor, which is a key achievement before 100 kg/day scale production. Products were successfully tested by external vendors to prove both the purity, low-toxicity, and antimicrobial performance. Multiple samples were sent out for trials with our partners, such as Gush/Livinwall and Kowa/Japan.

The team is currently now focused on completing 100 kg/day trials in CARES and planning large scale trials at a production facility in Malaysia in Q3. AMPLE has also been extended to the end of November 2024 to allow additional time for production scale trials to take place.

The commercial trajectory of AMPLE has also shifted in response to market demands and increasing conservativity from the investment market. Instead of constructing a multi-ton commercial facility in Singapore, which requires a capital investment of up to SG$20M, we are now focused on distributing our R&D and production technologies as a product platform. This includes software, hardware, services and licensing opportunities. This approach has already seen success with multiple requests for trials from partners. As AMPLE enters it's next phase, we are in due diligence discussions with investors for the commercialisation of the technology through the CARES spin-off from the C4T programme, Accelerated Materials, which was also founded by Dr Nicholas Jose in 2020.

AMPLE has also begun to expand its digital presence, by becoming involved in the CARES-hosted Pharma Innovation Programme Singapore (PIPS) project titled "From Digital Twins to Real Time AI-supported Plant Operation", which seeks to create a real time digital twin of the pilot production process. In this project, AMPLE members are assisting collaborators in CARES and Singapore's Agency for Science, Technology and Research (A*STAR) to create a user-friendly knowledge-graph tool for industrial use.

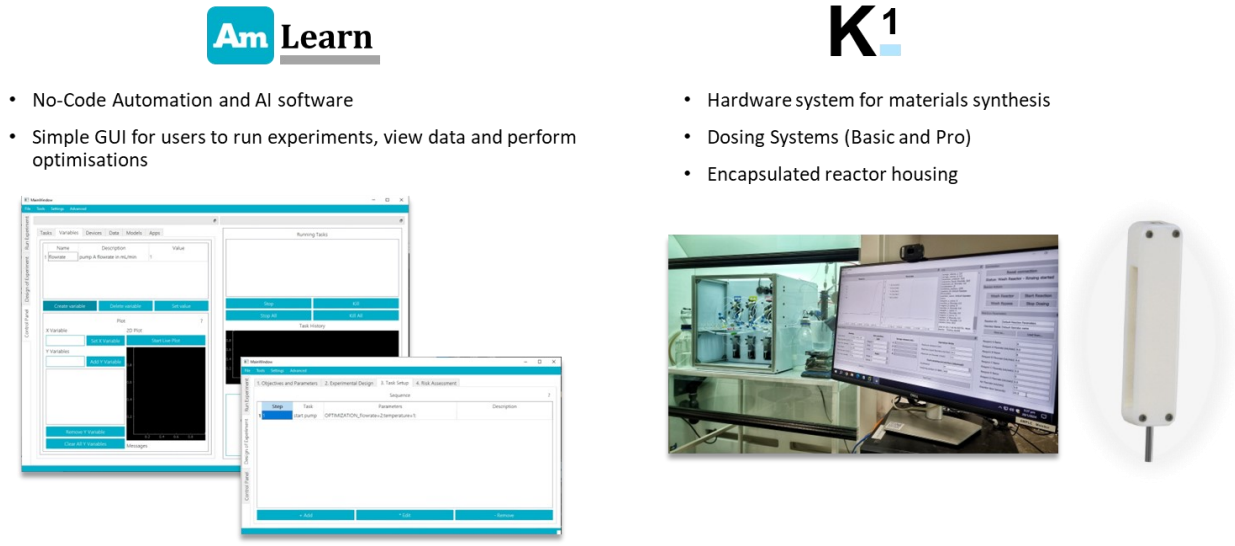
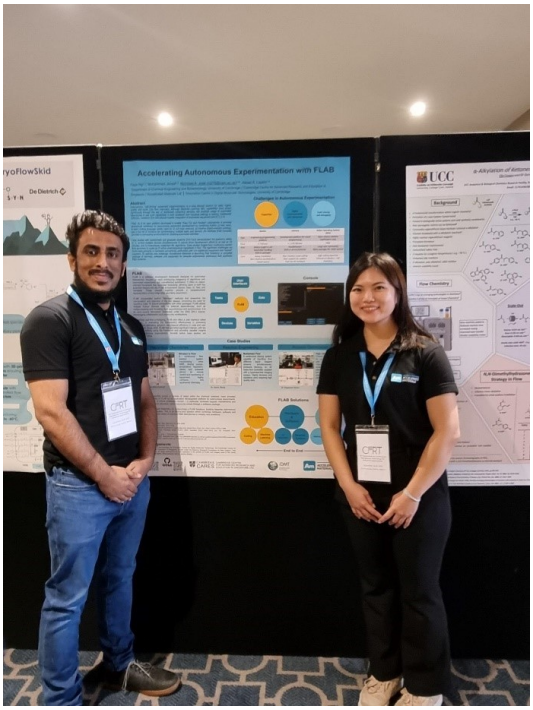


Figure 7.1: Product platform of software and hardware to be commercialised following AMPLE.

Other activities and achievements

AMPLE has signed an MOU with Kowa Co. Ltd. for trade show exhibition partnership at Nano-tech Japan 2024. Pictured in the bottom left photo are AMPLE members **Dr Susithra LAKSHMAN-AN (Chemical Engineer, AMPLE)** on the left, **Dr Nicholas JOSE (Project Lead, AMPLE)** on the second-left and **Mr Kelvin YEO (Business De-velopment Manager)** on the right.

Pictured in the bottom right are **Dr Mohammed JERAAL (Materials Engineer, AMPLE)** and **Ms Faye NG (Automation Engineer, AMPLE)** pre-senting a poster "Accelerating Autonomous Ex-perimentation with FLAB" at the 14th Symposi-um for Continuous Flow Reactor Technology for Industrial Applications from 27 - 28 September 2023 in Dublin, Ireland.



AMPLE continues collaborative work with Gush (LivinWall) in Singapore and Crown Paints in the UK for their antimicrobial ZnO particles. They are also working to implement their AI technologies for flow chemistry with Vapourtec, which they will exhibit at ACHEMA 2024 from 10 - 14 June 2024 in Frankfurt, Germany

AMPLE are engaging Evonik, Pfizer, KCTech, and NXMaterials as potential trial partners for their reactor and software technologies. They have also been engaging with Dymax in Singapore as a po-tential user for their additives.

AMPLE were recently awarded an APAC Business Development Initiative Grant through the UK-APAC Tech Growth Programme which will be used for business expansion.

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, and hence is ideally positioned to deliver this project.

During the period covered in this report, CDI has progressed in parallel work in three areas of the project: developing an ML model for predicting impacts of waste treatment processes, predicting inventories of synthesis routes to small medicinal molecules in the case when kinetic data is available, and automating assembly of synthesis paths to target molecules starting from compounds for which full life cycle inventories do exist. The project is progressing according to the plan and is in the phase of preparing the completion of its first milestone.

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 84)

During this reporting period, the modelling team is currently developing the schematic for the ontology-based digital twin method for the maintenance of physical models in chemical processes, as illustrated in Figure 8.1. This method would allow the rapid assembly of a suitable process model and its preparation for downstream tasks. The team has designed three ontologies: OntoModel for basic physical equations, OntoProcess for process description access, and OntoTask for modelling task information. OntoModel aims to encompass basic chemical process equations describing reactions, mass transfer, catalysis and mixing, thereby incorporating chemical engineering knowledge into the digital twins. When applied to detailed chemical processes, OntoProcess represents process phenomena and data access, and matches the process with physical equations. OntoProcess also assembles equations as a physical model, facilitating their use in model identification and calibration by OntoTask.

As shown in Figure 8.2, one practical application of this ontology-based digital twin method is to model the annular reactor and quantify its performance in stream mixing. In the annular reactor, engulfment mixing is identified as the mixing mechanism for streams, sheared by the gas flow in the tube. The mixing time, a parameter indicating the efficacy of stream mixing, is calibrated using the automatically assembled physical model when the gas flow rate changes.

The ontology team collaborated with the implementation team to develop codes facilitating smooth data exchange between AMPLE's Kepware Open Platform Communications Unified Architecture (OPC-UA) server and Microsoft Azure Internet of Things (IoT) Edge, which is necessary for creating a real-time digital twin of AMPLE's pilot plant on the Microsoft Azure platform. A workflow for connecting AMPLE's Kepware OPC-UA server to I²R Microsoft Azure IoT Edge has been developed, which includes establishing reliable connectivity and data exchange

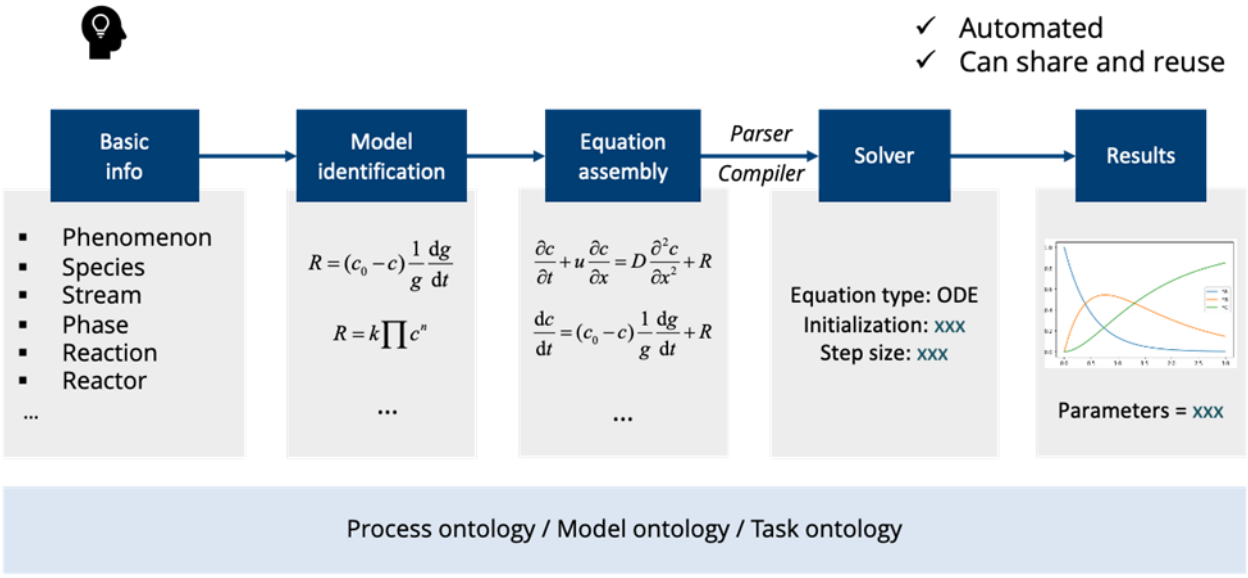


Figure 8.1: Workflow of the physical model formulation using the ontology-based digital twin method. Starting with collected basic information, the method is designed to automatically assemble equations and propose physical models that can be shared and reused for modelling maintenance.

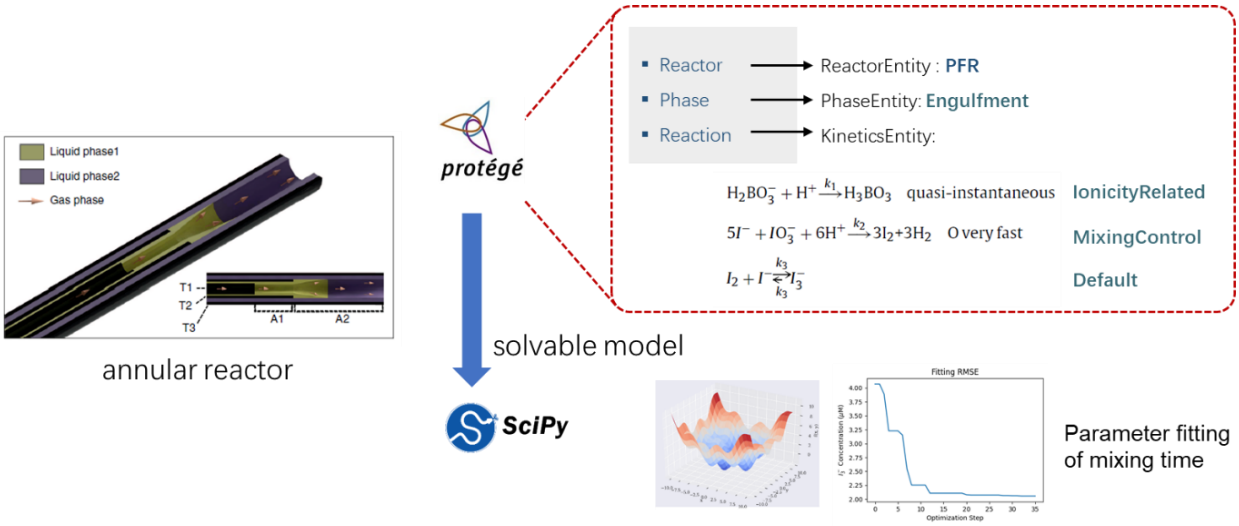


Figure 8.2: Application of the ontology-based digital twin method to the annular reactor. The plug flow reactor and engulfment mixing are identified as the reactor and mechanism for phase mixing, respectively. Kinetics for the respective reactions are also analysed. The automatically derived solvable model is then optimised to fit the model-parameters.

among various devices within AMPLE's pilot plant and with Microsoft Azure IoT Edge, and defining the requirements for connecting to I²R Microsoft Azure IoT Edge, such as specifying file formats and properties. Figure 8.3 illustrates the four steps for establishing connectivity from the AMPLE Kepware OPC-UA server to the I²R Microsoft Azure IoT Edge.

The first step involves developing and extending ontologies to represent devices and their associated parameters and data within the knowledge graph. The second step entails understanding the requirements for data and file formats to be sent to the Microsoft Azure IoT Edge. Following discussions with the implementation team, a combination of .DTDL and .XLSX files has been identified by the implementation team as the compatible file combination for creating the ontology on the Microsoft Azure platform. Subsequently, the third step consists of creating a converter to transform ontology instances from the Web Ontology Language (OWL) format to Microsoft Excel Spreadsheet (XLSX) format. The final step involves writing code to extract relevant data from the AMPLE Kepware OPC-UA server and update ontology instances with the extracted data.

Additionally, the ontology team implemented secure data access to AMPLE's Kepware OPC-UA server, ensuring credential based access only. A Virtual Private Network (VPN) connection was explored, but not utilised due to errors encountered during installation and unsuccessful troubleshooting after consultation with the technical team. The team also started the development of workflows and codes to manage time series data retrieved from AMPLE's Kepware OPC-UA server onto the Microsoft Azure platform.

Furthermore, several ontologies were developed and extended to represent selected devices, their associated parameters, and data within the knowledge graph for the dosing module of AMPLE's pilot plant. These ontologies were developed based on the plant process flow diagram and Kepware OPC-UA server variables provided

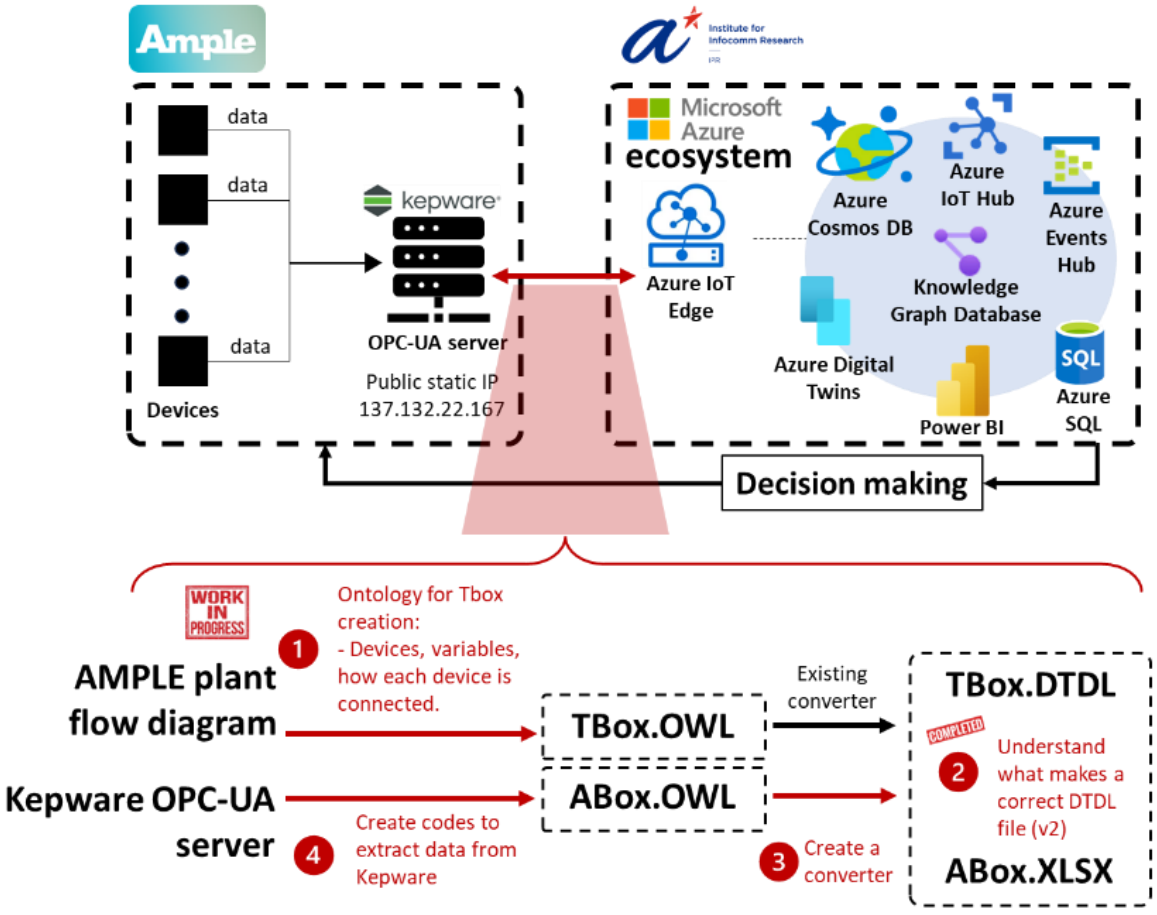


Figure 8.3: Snippet of workflow for connecting AMPLE Kepware OPC-UA server to I²R Microsoft Azure IoT Edge.

by the AMPLE team, leveraging existing ontologies such as OntoDevice (represents devices), OntoBMS (represents the Building Management System components), OntoCAPE (represents the domain of Computer-Aided Process Engineering), Ontology of Units of Measure, SAREF (represents smart devices and applications), and s4bldg (SAREF extension for buildings). A snippet of the ontology, focused on the Compressed Dried Air Line of the dosing module is shown in Figure 8.4. Currently, the team is developing ontologies to represent the reactor module within AMPLE's pilot plant in the knowledge graph.

On 24 January 2024, the entire team engaged with the AMPLE team in an internal workshop to discuss and refine project deliverables, including defining the proof-of-concept demonstration. During the workshop, pain-points faced by the AMPLE team in their daily operations with the pilot plant were revealed. Based on these pain-points, several use cases were identified that aim to address the issues. Some of the use cases include: automated recording of data from trial synthesis through the integration of online and offline data, prediction and detection of system faults, and real-time digital twin representation.

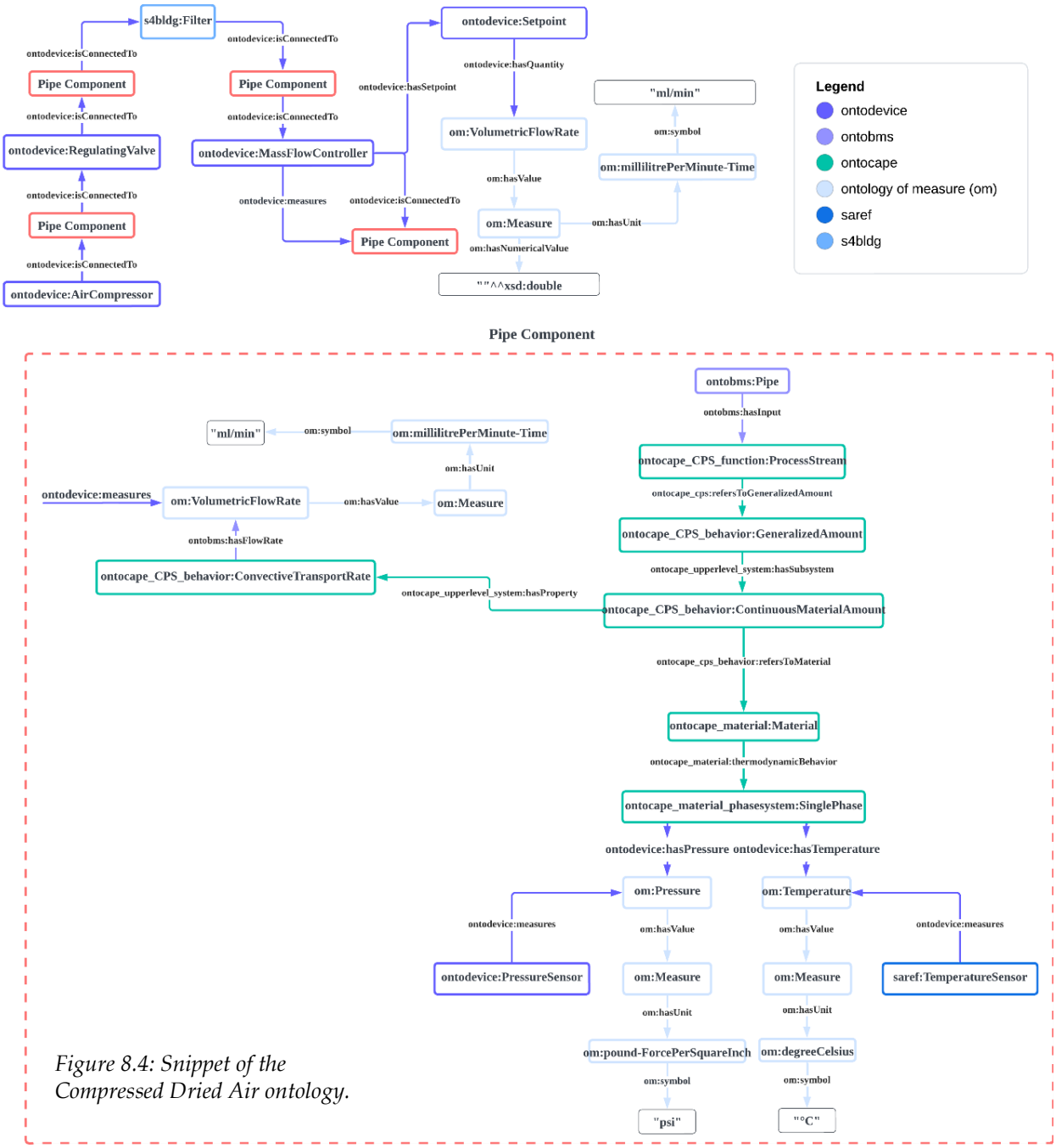


Figure 8.4: Snippet of the Compressed Dried Air ontology.

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 Knowledge Graph Driven P2P Energy Trading and Real-time Network Operation for High Renewables (an Intra-CREATE seed collaboration grant), and contribution towards Cooling Singapore 2.0 hosted by the Singapore-ETH Centre.

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.

Knowledge Graph Driven P2P Energy Trading and Real-time Network Operation for High Renewables

Intra-CREATE seed collaboration grant

The project aims to develop an energy market framework that leverages the benefits of a dynamic knowledge graph for efficient peer-to-peer (P2P) energy trading between prosumers while satisfying the stable and secure operation of the distribution grid. The 18-month project will end in March 2024.

During this reporting period, **Dr Casper LINDBERG (PI, CARES)** and **Mr Mingchuan TIAN (Software Developer, CARES)** worked on enriching The World Avatar base world with details from NTU and improving the visualisation. Dr Lindberg integrated peer-to-peer (P2P) trading, Bubble Neural Network, and control algorithms developed by the NTU team as computational agents in the knowledge graph. He implemented these algorithms as Python agents within the NTU Digital Twin Docker stack, creating SPARQL queries to allow the agents to query and update data in the knowledge graph, and updating the visualisation to display the agent output. This work will complete the implementation of a framework that allows for the calculation, visualisation, and control of voltage levels across the network, featuring P2P energy trading and solar production. Dr Lindberg is currently writing up this work for publication.

Mr Tian instantiated historical data from water stations in NTU into the knowledge graph and visualised them to facilitate environmental monitoring within the existing system. He developed an ontology to represent water quality metrics for this purpose. He also integrated a Grafana-based interactive dashboard into the NTU Digital Twin to visualise complex datasets, including class schedules, water monitor readings, and power consumption data, in a more user-friendly manner.

Figure 9.1: Example of heat maps visualising voltage levels before (previous page) and after (current page) a control action. Red indicates areas of overvoltage and green represents nominal voltage.

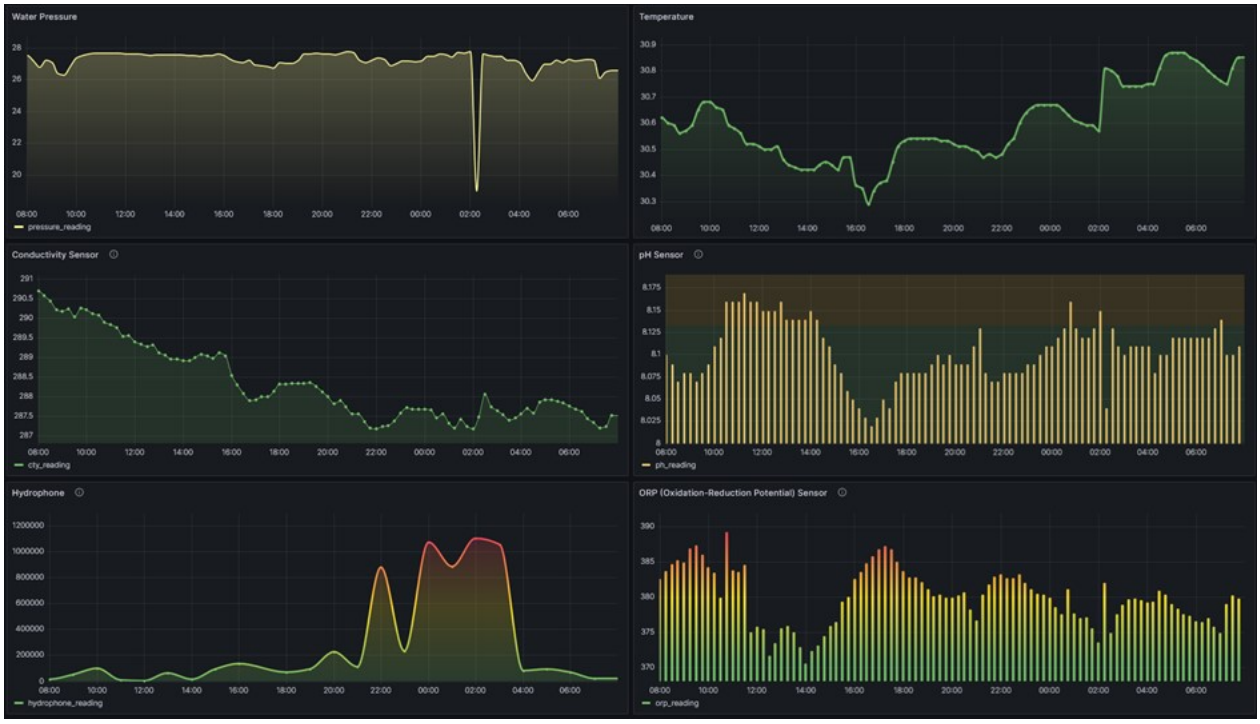


Figure 9.2: Grafana-based interactive dashboard visualising water monitor readings.

Dr Hung NGUYEN (PI, NTU) and Dr Veerapandiyan VEERASAMY (Research Fellow, NTU) worked on a fuzzy clustering approach to train the Bubble Neural Network for identifying buses belonging to over and under voltage groups. They assisted Dr Lindberg in wrapping this as a computational agent in the knowledge graph to categorise the buses based on their voltage levels. Furthermore, Dr Nguyen and Dr Veerasamy designed a control action using reinforcement learning techniques to improve the probability of buses remaining within the nominal voltage region rather than experiencing over or under voltage. They also developed a P2P trading framework using Alternating Direction Method of Multipliers (ADMM) techniques to enable knowledge graph-driven P2P energy trading. Dr Nguyen and Dr Veerasamy successfully tested the framework on the IEEE 14-bus system at NTU, while Dr Lindberg tested the same framework on the 15 -bus test system at NTU. Dr Nguyen and Dr Veerasamy are currently writing a journal article to publish these results.

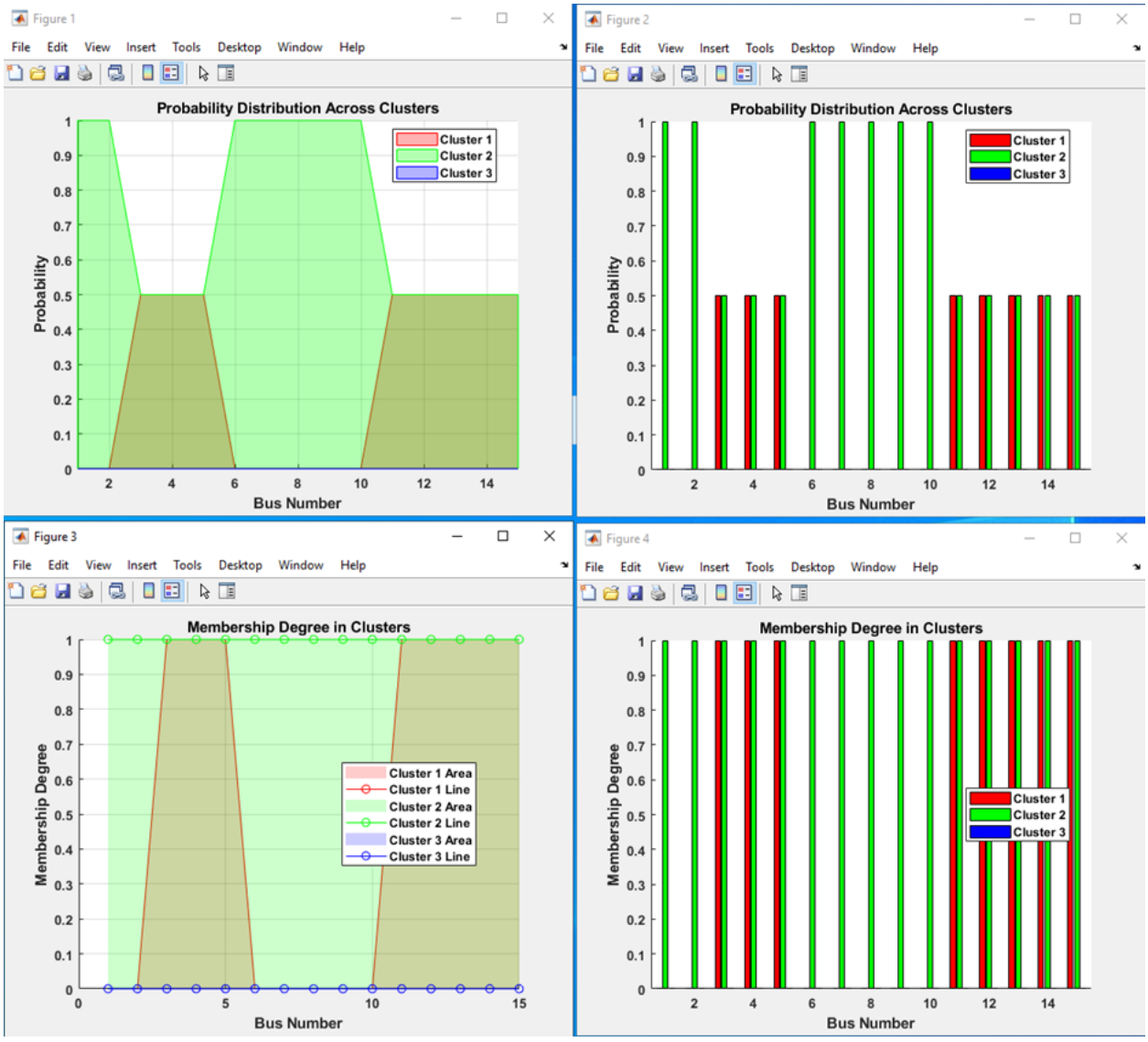


Figure 9.3: Probability distribution of the NTU test system for various cases.

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 Jurong Island, Singapore, by developing computational energy models using The World Avatar (TWA). The results of these models constitute the input for DUCT. CARES will also perform sensitivity analysis to investigate the impact of anthropogenic heat emissions from industrial activity in Jurong Island on Singapore. As part of the work under the Cooling Singapore 2.0 project extension, CARES is also estimating anthropogenic heat emissions from various industries on Singapore mainland.

Dr Karthik NAGARAJAN (Software Developer, CARES) has evaluated a number of scenarios involving variations in the estimated heat emissions, heights and locations of the identified heat sources, summarised as follows:

- Setting the estimated emissions rate of each identified heat source to 23.5% of the baseline value to account for differences with the officially reported values of proxy indicators and the Singapore Green Plan 2030.
- Increasing the estimated emissions rate of each identified heat source by a factor of 2 compared to the baseline as the estimated minimum utilisation rate of chemical plants and refineries is reported in the literature to be approximately 50%.
- Setting the estimated heights of all identified heat sources to 2 meters, representing the minimum height of identified heat sources in Jurong Island.
- Setting the estimated heights of all identified heat sources to 150 meters, representing the maximum height of identified heat sources in Jurong Island.
- Moving all identified heat sources to a single grid cell located on the coastline of Jurong Island adjacent to the Singapore mainland. The locations are chosen such that the nearest point on the Singapore mainland is 1.3 – 1.5 kilometers away. The former value represents the minimum distance between two points in Jurong Island and Singapore mainland.

The primary metric used to assess the temperature impact of estimated anthropogenic heat emissions from Jurong Island is the quantity ΔT_a, defined as $\Delta T_a = T_a - T_r$. Here, T_a denotes the average temperature in a region of interest in the presence of identified industrial heat sources, while T_r denotes the corresponding average temperature in their absence. All regions for which T_a was evaluated have dimensions of 1,500 × 1,500 meters. All simulations were run for a 24-hour period corresponding to 18 April 2016, using DUCT's mesoscale climate module. The values of ΔT_a ranged between -1.55°C and 0.66°C for all tested cases and were found to be within the uncertainty range of the model.

Figure 9.4 (left) shows the corresponding spatial temperature distribution in the absence of industrial heat sources for reference. The maximum positive temperature impact of 0.66°C occurs when the estimated heat emission rate of each identified heat source is set to double the baseline value. The spatial temperature distribution for this case is shown on the right side of Figure 9.4. The total estimated heat emission rate of all identified heat sources in the baseline scenario is denoted as Q. The region with the maximum positive temperature impact is indicated by the red rectangle.

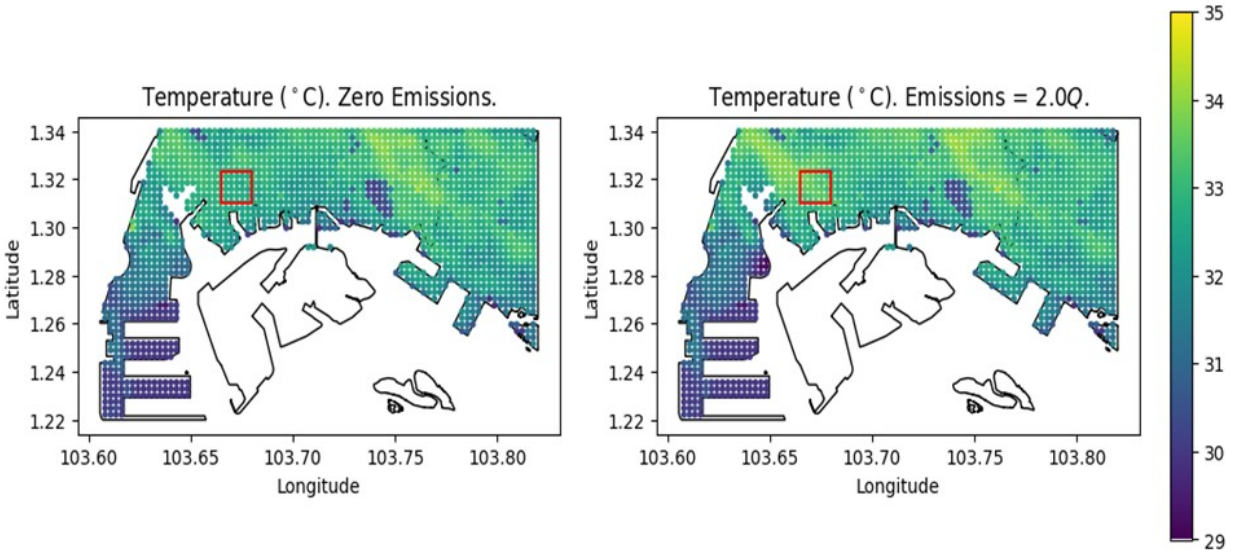


Figure 9.4: Spatial temperature distribution for zero industrial heat emissions (left) and with estimated heat emissions rates set to double the baseline value, 2.0Q (right). The region with the maximum positive temperature impact is indicated by the red rectangle.

Currently, Dr. Nagarajan is estimating the heat emissions of various industries in Singapore mainland. Some preliminary data have been obtained for the chemicals, data centers, semiconductors and food industries. He is currently collecting additional data to improve the estimation of the heat emissions for various companies in these industries and to perform similar estimations for the precision engineering, pharmaceutical, and printing industries. He has also developed an OntoCompany ontology that contains classes such as "Factory" and "DataCentre" and relations such as "hasDesignCapacity" and "hasSpecificEnergyConsumption" to semantically represent the companies' attributes in a knowledge graph.

Dr Nagarajan presented the poster "Estimation of heat emissions from industries in Jurong Island and their temperature impact" in November 2023 to Digital Urban Climate Twin (DUCT) users from various government agencies.

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