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A research collaboration platform:
University of Cambridge
and Singapore

Biannual Research Report April - September 2026



COVER IMAGE

Group photo taken during Lord Chris Smith's first visit to CARES as University of Cambridge Chancellor, featuring (from left) CARES Chief Operating Officer Elizabeth MacRae, Dr Vibhuti Patel, Prof Grant Stewart, Lord Chris Smith, CARES Director of Industrial Relations Prof Epaminondas Mastorakos, Prof Jean Abraham and CARES Director of Education and Skills Prof Henriëtte Hendriks.

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CLIC, HYCOMBS, SM_3, HD_4, NH_3-SOFC and eCO_2RR are supported by the National Research Foundation, Prime Minister's Office, Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) programme.

Building a Capacity in Magnetic Resonance Methods for the Pharmaceutical and Agrochemical Sector within PIPS is supported under the Pharmaceutical Innovation Programme Singapore.

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

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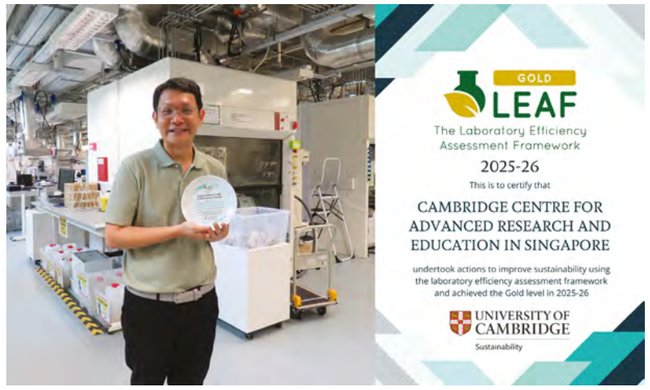
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Foreword

CARES can identify that the busiest and most photographed item of interest in the last six months is our laboratory in the CREATE building.

Our lab was recently awarded a Gold LEAF (Laboratory Efficiency Assessment Framework) recognition for improved sustainability practices since tracking started in 2023, the most notable being a near-half reduction in electrical and chilled water consumption. We acknowledge this effort in huge part to the lab technicians, contractors, and researchers for committing to change daily habits, reporting anomalies, and conducting long-term equipment monitoring.





The lab has since hosted visitors ranging from French students on a knowledge exchange visit to international delegates from New Zealand's Business, Innovation and Employment Programme learning about the positive impacts of research funding on business and talent development. In April 2026, CARES had the delight of hosting the Chancellor of the University of Cambridge, Lord Chris Smith, on his first international trip in his new role. Lord Smith spent time meeting our researchers and viewed several lab demonstrations.



Lastly, Channel News Asia featured the lab in a recent documentary, *Breakthroughs: Race for Green Seas*, as the testbed for improving electrochemical devices and making green hydrogen production more efficient. While public outreach naturally gravitates towards researchers and novel ideas, these last six months have shown a rightful spotlight on the cutting-edge research equipment that CARES maintains to develop our technologies.

CARES' first healthcare project, BloodCounts!

BloodCounts! will use AI to analyse the commonly discarded data from a complete blood count test to expand its diagnostic capabilities for a wide range of diseases. The project started within the University of Cambridge with UK hospitals, and expanded to include Consortium members from various continents, and now Singapore. CARES is delighted to host the new Singapore-specific research with local hospitals SingHealth and National University Health System (NUHS) as a project under the new AI-for-Science (AI4S) initiative.

Combustion scientists are working with the industry

The Hydrogen and Ammonia Combustion in Singapore (HYCOMBS) researchers had a busy April with industry-facing events. The team had a booth at Singapore Maritime Week 2026 (a consecutive three-year occurrence for CARES now!) to share our research with technology providers, policymakers, and business analysts. The subsequent HYCOMBS School was an organised 2-day event to share our latest research with academic members and industry engineers of the combustion community.

CARES @ CREATE Symposium 2026

CARES joined our CREATE community to contribute a speaking session and a booth at CREATE Symposium 2026. Under the Symposium's theme "Climate, Environment, Health and Urban Resilience," Prof Nick Wareham from our Health-driven design for cities (HD4) programme highlighted how HD4's partnership with the SG100K study will enrich the evidence-based relationship of the environment's influence on human health outcomes in Asian cities. The booth provided a chance for CARES to network with other CREATE programmes, with many researchers discovering common themes in their work.

Please get in touch with us if you would like to know more about our work or have ideas for collaboration.



About Us

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

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

The first programme administered by CARES, the Cambridge Centre for Carbon Reduction in Chemical Technology (C4T), wrapped up in October 2025 after 12 years. The motivation for C4T was to provide a rich pipeline of scientific insight and technological innovation with high potential for positive results within the decarbonisation agenda if deployed by appropriate industry and government parties.

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

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

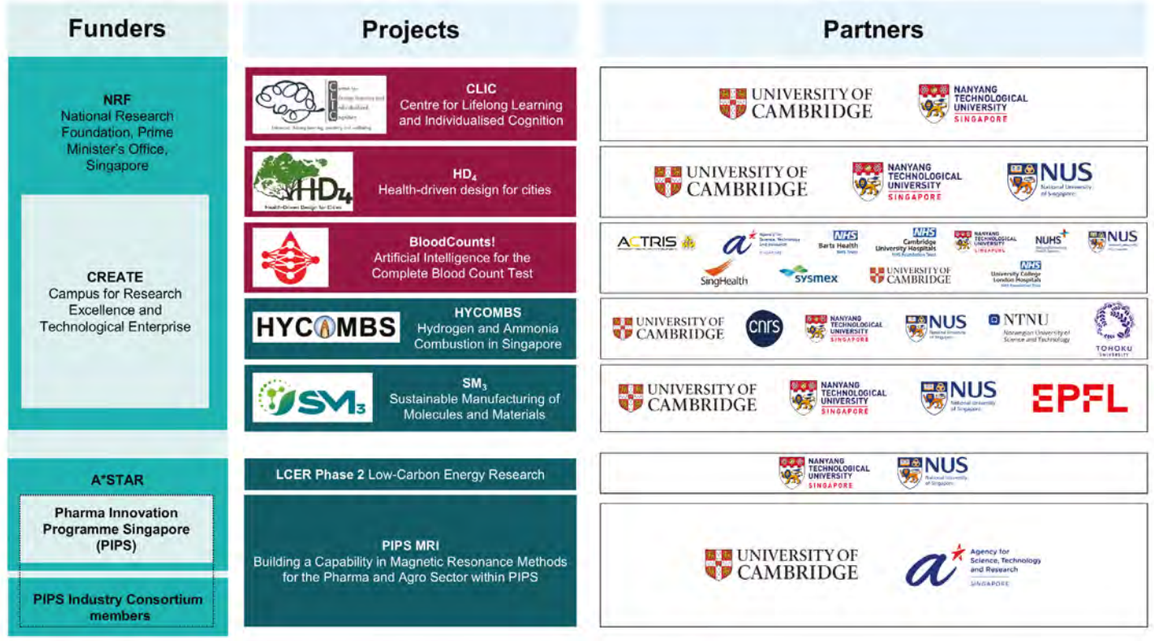
C4T's impact and contribution to fundamental research (726 papers and an H-index of 106 to date), technology development (36 invention disclosures, 52 patent filings and 4 licenses), and translational impact (6 spin-off companies), is evident. The programme has also hosted 47 PhD students, some with matched industry funding through the Cambridge-CARES studentship scheme. As C4T ends, we celebrate the programme's legacy and platform for kickstarting our new decarbonisation projects.

In July 2024, NRF announced a new SGD$90m Decarbonisation programme. The two CARES-hosted project under this initiative are Hydrogen and Ammonia Combustion in Singapore (HYCOMBS), and Sustainable Manufacture of Molecules and Materials in Singapore (SM_3). New collaborators on these projects include Tohoku University, CNRS, the Norwegian University of Science and Technology, and the Swiss Federal Technology Institute of Lausanne.

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

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

The start of BloodCounts! in June 2026 adds to the portfolio as CARES' first project in healthcare that converges with AI research. BloodCounts! will build frontier AI models to reveal new patterns from the complete blood count (CBC) and create opportunities for earlier disease detection in Singapore and worldwide.



The Pharmaceutical Innovation Programme Singapore (PIPS) will use magnetic resonance imaging to optimise operating conditions for heterogeneous hydrogenation reactions in continuous-flow microscale trickle-bed catalytic reactors.

CARES is also contributing to a project under the Low-Carbon Energy Research (LCER) Phase 2 Programme, and a sub-awardee in two projects under the CREATE Thematic Programme in Decarbonisation, these are "Decarbonization with Green Ammonia Using solid Oxide Fuel Cell (SOFC) for Power Generation" and "Development of Advanced Catalysts for Electrochemical Carbon Abatement".

CARES celebrated its first decade in Singapore in 2023 with a Scientific Showcase highlighting achievements in Digital Transformation, Chemical Technologies and Processes, From Emissions to Solutions, and Lifelong Learning. The scientific content from the event and highlights from 2023 can be viewed on our website.

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









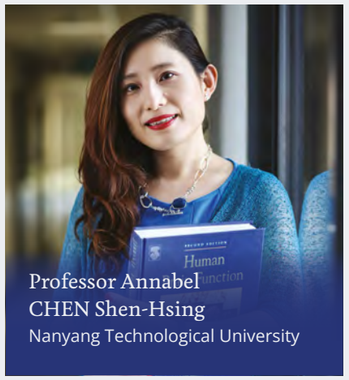


CLIC

CENTRE FOR LIFELONG LEARNING AND INDIVIDUALISED COGNITION

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

Directors



Professor Annabel CHEN Shen-Hsing
Nanyang Technological University



Professor Zoe KOURTZI
University of Cambridge

CLIC has made substantial progress across its three Work Packages during the reporting period, advancing both the scientific understanding of cognitive flexibility (CF) and its translation into educational and real-world contexts.

The team has progressed the SLiCX intervention from platform development into active participant testing. The team successfully launched Airship, a dedicated testing platform, in April 2026, with 54 participants recruited into the study to date. In response to SAC recommendations, the team developed a more engaging, gamified Structure Learning (SL) task and developed a modified *All You Can E.T.* active control condition, in collaboration with the NYU-CREATE team. The neuroimaging component has also progressed, with multimodal acquisition and analysis pipelines established. Preliminary findings indicate intervention-specific changes in prefrontal neuroplasticity, although these findings remain exploratory given the ongoing recruitment and current sample size. The team has also advanced research on the emergence of CF in early childhood and the development of neuropersonalised brain stimulation approaches to enhance learning.

Work Package 2 has continued to broaden the understanding of how cognitive flexibility relates to language learning, social factors, and career development. The team has successfully published three peer-reviewed papers (Sam et al., 2026; Feng et al., 2026; Feng et al.,2026) during the current reporting period and have also presented their collaborative findings on multilingualism and CF at the 2026 International Society for the Study of Behavioural Development (ISSBD) meeting in South Korea. The Language Learning study has recruited 198 young adults and has established a collaboration with inlingua School of Languages to strengthen their recruitment efforts to engage with working adults enrolled in language courses. The Social Framing study has received IRB approval, while the Career Study is undergoing IRB review.

In the last six months, the CLIC team has focused on developing scalable approaches for assessing and applying CF in adolescent and educational settings. The team has developed a shortened Structure Learning Lite (SLite) protocol and streamlined the Crossing Valley and colour-shape tasks to reduce testing time and improve feasibility in schools. The Scientific Reasoning Task was also revised and piloted, with preliminary findings indicating that the shortened versions retain expected associations with key CF measures. Chiefly, the team has continued to strengthen translation into practice through quarterly engagement with the Ministry of Education and an expanding partnership with the Singapore Examinations and Assessment Board (SEAB). This included a keynote and CF workshop at the 2026 SEAB Assessment Conference, which reached approximately 950 educators, as well as continued joint work on the application of CF research to educational assessment and pedagogy.

Altogether, the current reporting period has seen CLIC progress from intervention development and foundational research towards active testing, validation, and translation. Across the Work Packages, the programme is increasingly focused on developing scalable and ecologically relevant approaches to understanding, assessing, and strengthening cognitive flexibility across the lifespan, while building and maintaining sustained partnerships with policymakers, educators, and external research collaborators.

Professor Annabel Chen Shen-Hsing
Director of CLIC, NTU

Professor Zoe Kourtzi
Director of CLIC, CAMBRIDGE



WORK PACKAGE 1

Since the last update, the team has made steady progress in the last six months. This includes the launch of Airship, a dedicated Structure Learning-based Cognitive Flexibility Training Suite (SLiCX) testing platform, in April 2026. The SLiCX team held an in-person, internal training workshop in May 2026 which served as a refresher course for all staff involved in recruitment, as well as familiarising the wider CLIC team with SLiCX procedures ahead of data collection. The Airship platform onboarded its first participant in May and 54 participants have been recruited to SLiCX, with 37 having completed the study.

In response to recommendations from the Scientific Advisory Committee (SAC) to strengthen engagement and reduce attrition, the team has developed a gamified version of the Structure Learning (SL) task. This new version incorporates an interactive exploration-style environment, visual characters, progressive levels, and rewards for successful task completion, while retaining the core cognitive demands of the SL paradigm. The task has been designed to align as closely as possible with the game-based format of the active control condition. To support engagement, the experimenter guides participants through the storyline using live narration as events unfold, creating a more immersive experience while maintaining standardised administration. The team has been working closely with the NYU-CREATE team to develop and establish *All You Can E.T.* (AYCET) on the NTU server and adapt it for the SLiCX protocol. The task was successfully configured and ready for participant testing in July 2026.

Following recommendations from the Ministry of Education (MOE), the adolescent component has been separated from SLiCX and will be developed and validated as a shortened SL intervention. A detailed progress update is described under Work Package 3.

The SLiCX neuroimaging component is progressing well, with multimodal acquisition protocols established and analysis pipelines implemented across imaging modalities and the MRI SL task. The team has refined the imaging protocols to strengthen the study design, with preprocessing and analysis pipelines now established and applied. Based on consultations and recommendations from the SAC, MOE and the National Research Foundation, the team has similarly shifted efforts to focus on the adult population. Preliminary imaging and behavioural analyses indicate intervention-specific prefrontal neuroplasticity, with distinct neurochemical changes following AYCET and SL training. These findings remain exploratory given the current sample size (mean age: 25.38 ± 2.17years, range: 21.38–29.62, control (n=17), AYCET (n=16), and SL (n=8) groups), as participant recruitment to the SLiCX study is still ongoing.

Beyond SLiCX, CLIC continues to investigate the development of cognitive flexibility across the lifespan, including its relationship with creativity, school readiness, and early social contexts. A pilot study involving children aged 12–48 months is underway, integrating EEG and ECG measures to examine the neural and physiological mechanisms underlying emerging cognitive flexibility and creativity, as well as the social contexts that support their development.

Building on the Cambridge–NTU team's demonstration that visual flicker-based neuropersonalised entrainment can improve adult perceptual learning (Michael et al., 2022, Cerebral Cortex), the protocol has been successfully adapted for non-invasive brain stimulation. A Cambridge pilot study involving 60 adults used transcranial magnetic stimulation (TMS) and concurrent EEG to entrain parietal alpha oscillations during a perceptual learning task. Participants showed significantly improved and sustained perceptual performance when stimulation was matched to their individual alpha frequency, compared with non-matched stimulation. CLIC Singapore team members are currently being trained to replicate the TMS neuropersonalisation protocol in a structure learning task, while technical testing is underway to produce stimulation pulses at the requisite frequency with high fidelity.



Top left: Prof Henriëtte Hendriks presenting an overview of CLIC to the Chancellor of Cambridge, Lord Chris Smith during his visit to CARES in April 2026. Top right: Lord Chris Smith a trying out a game for Structure Learning used in CLIC's participant studies. Bottom photos: Prof Annabel Chen interacting with the delegates.

WORK PACKAGE 2

During the reporting period, the team published three papers. These include a paper examining measurement issues in the Big Five Inventory published in the European Journal of Personality; a study on behavioural game theory tasks published in Behavior Research Methods; and a study evaluating the Career Construction Model of Adaptation (CCMA; Savickas & Porfeli, 2012) published in *Frontiers in Psychology*.

The team has made steady progress across the ongoing intervention studies investigating language learning, social framing, and career development. For the Language Learning study, 198 young adult participants have been recruited. The team has also reached out to external collaborators, including the inlingua School of Languages to support recruitment of working adults enrolled in a language course. Meanwhile, the questionnaire batteries, study design, and task programming for the Social Framing study have been finalised, and the adult study has received IRB approval. The Career Study has also progressed across several key areas. The study examines the effectiveness of different career intervention formats (i.e., static Q&A versus an interactive, digitally guided approach) and whether the framing of the exercise influences career-related outcomes. IRB application is currently under review.

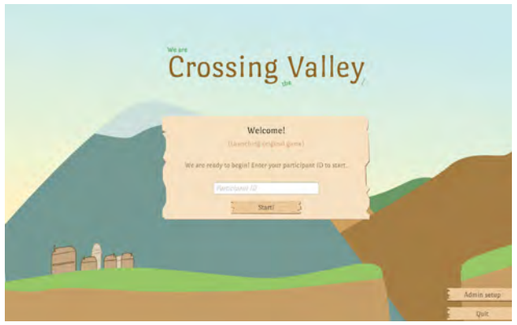
The team is also preparing three additional manuscripts: (1) the relationship between language entropy and cooperativeness; (2) associations between multilingualism and cognitive flexibility across adolescents and adults; and (3) the relationship between self-reported and task-based cognitive flexibility, including how these measures relate to core executive functions such as working memory and inhibitory control.

WORK PACKAGE 3

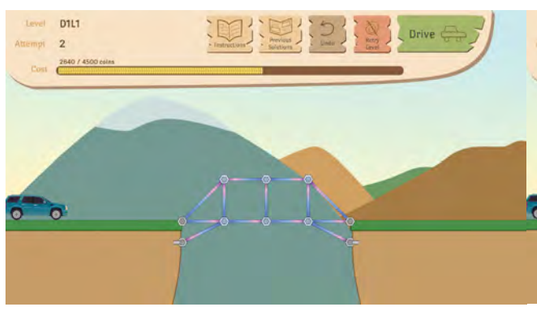
The team has continued to refine and validate its adolescent task batteries for both structure learning and the Critical, Adaptive and Inventive Thinking (CAIT) paradigms, with a focus on developing a shorter version of the battery for adolescents. The team has been working on balancing engagement and fatigue associated with lengthy cognitive testing, which is crucial to improving scalability in classroom settings, given the limited curriculum time and teaching resources available in schools.

The structure learning intervention training requires multiple consecutive days of 30-minute sessions. While the results for SL for adults have been encouraging, the time commitment for SL poses significant implementation challenges for adolescents and schools. The team has reconceptualised SL as a potential cognitive flexibility profiling tool and has developed a validated shorter version – Structure Learning Lite (SLite). This builds on promising findings that an individual's cognitive flexibility profile could be predicted through early performance in SL. SLite consists of two days of cognitive testing, with a 10-minute structure learning session each day alongside other cognitive tasks. SLite could potentially be used to develop cognitive flexibility profiles and inform tailored cognitive flexibility training if its predictive performance and strategy indices are supported. Concurrently, the team is working with WP1 to explore ways of improving engagement, as adolescents continue to find SL challenging to engage with, despite its shorter format.

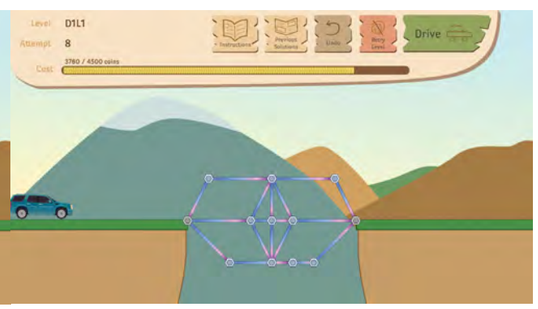
The Crossing Valley bridge-building game was further streamlined following its 2025 pilot. The task was originally designed to examine how participants adapt their strategies under changing conditions, including bridge lengths, vehicle weights, and budget constraints. The levels have now been refined across different difficulty levels, halving play time from 30 minutes to 15 minutes. Validations are ongoing to explore whether the shortened version is comparable to the original. Concurrently, the team is validating a shortened version of the colour shape task, administered as part of the Crossing Valley task battery, which has been reduced from 12 minutes to 7 minutes.



Crossing Valley homepage.



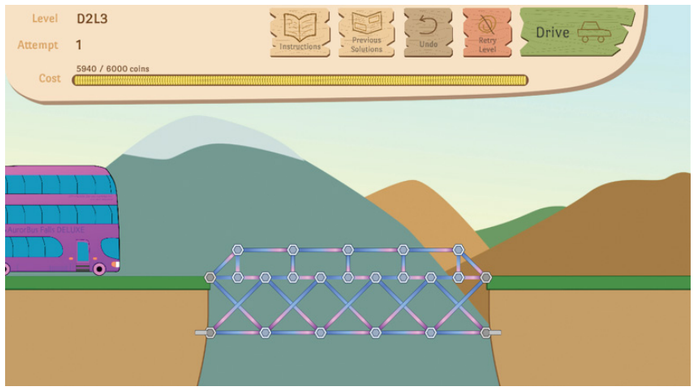
Bridge built by a player on the first level after the tutorial.



Same level as the photo on the left, but a different solution from another player.

The team revised the Scientific Reasoning Task (SRT), which investigates how naïve belief and scientific reasoning interact, and how CF may support the suppression of naïve responses. The revised task balances statements in each domain (math, biology, physics) to match Singapore's science and math curricula. This allows the team to investigate the timing of first learning a concept, the impact on the suppression of naive thinking and how cognitive flexibility supports this process. These revised studies were tested through several rounds of small-scale studies between June and August 2026. Preliminary analyses indicated that the condensed task versions maintained hypothesised correlations with key cognitive flexibility measures, with further analysis planned to validate these associations.

Apart from fine-tuning the research, WP3 has also continued engaging with policymakers, educators and the public. The team meets MOE on a quarterly basis (February, March and August 2026) to maintain alignment of expectations and its translation into practice.



Each level features changes in required bridge length and/or weight of the vehicle. The allocated budget for the bridge could also become an unexpected constraint for the player.

OTHER ACTIVITIES AND ACHIEVEMENTS

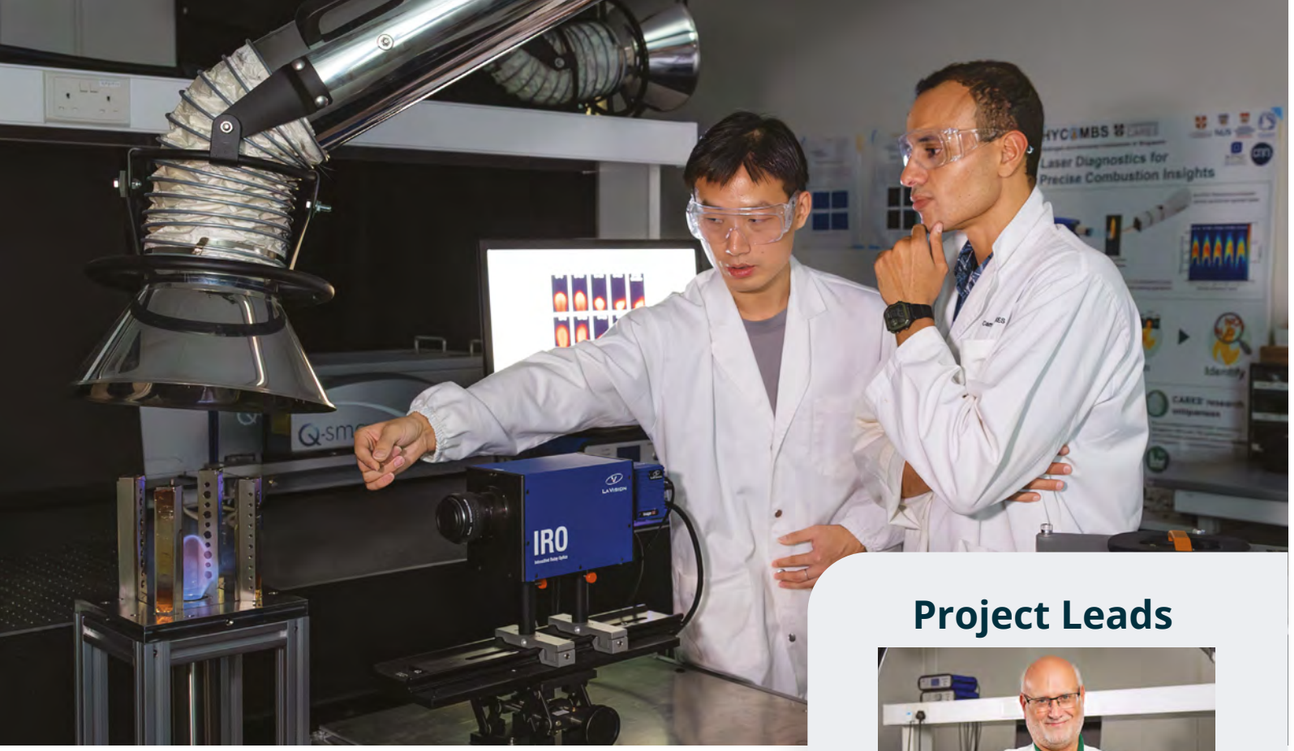
Work Package 3 researchers presented at the 28th Biennial Meeting of the International Society for the Study of Behavioural Development (ISSBD) from 21-25 June 2026 in Incheon, South Korea.

Dr Chew Lee TEO (Co-I, NTU) was invited as a keynote speaker at the Singapore Examinations and Assessment Board (SEAB) Assessment Conference 2026 on 29 - 30 April, which brought together approximately 950 primary and secondary school educators. Her keynote focused on knowledge building, cognitive flexibility, and their links to 21st-century competencies. The team also ran a cognitive flexibility workshop, engaging over 100 participants across both days. In July, the team returned to SEAB to share a more detailed analysis of the relationship between cognitive flexibility and the Critical, Adaptive and Inventive Thinking (CAIT) task.



Attendees at SEAB Conference 2026.

Ms Selvira MELIA (Research Assistant, NTU) and Dr Nastassja LOPES FISCHER (co-PI, NIE) presented a poster, "Adolescent Verbal Search Strategies: Implications for Cognitive Flexibility and Instructional Design", at the Redesigning Pedagogy International Conference (RPIC) from 2 - 4 June 2026 in Singapore on the links between executive function and cognitive flexibility performance with non-traditional verbal fluency outcomes. The results from hierarchical regressions and network analyses had implications for differing organisations of semantic memory among adolescents, which could suggest that instructional design may benefit from integrating mixed practice approaches.



HYCOMBS

HYDROGEN AND AMMONIA COMBUSTION IN SINGAPORE

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

Project Leads



Professor Epaminondas MASTORAKOS
University of Cambridge



Assoc Professor Fei DUAN
Nanyang Technological University



Professor Kaoru MARUTA
Tohoku University

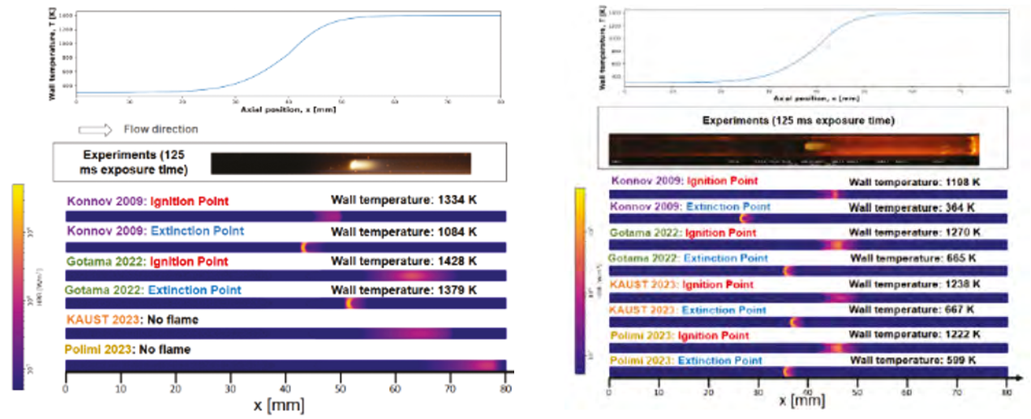
WP1: CHEMICAL KINETICS

Work Package 1 focuses on investigating the fundamental chemistry of the combustion of hydrogen, ammonia, hydrocarbons, and their blends. In this reporting period, we have completed the commissioning of the micro flow reactor (MFR) rig and its diagnostic systems. Ab initio calculations of rate coefficients for key nitrogen-combustion pathways, and systematic comparison of existing kinetic mechanisms against experimental and numerical benchmarks are ongoing to further the progress in the work package toward validated, reduced schemes for ammonia and hydrogen oxidation chemistry.

Chemical kinetics of combustion and pollutant generation

The 2D direct numerical simulation MFR code, developed using PeleLMeX, was tested against multiple chemical kinetic mechanisms. Given the wide variation observed among the results produced by these mechanisms, experimental validation (carried out in collaboration with Tohoku University) was performed to assess and rank their relative performance.

Comparisons were performed for ammonia/air (Figure 1.1(a)) and ammonia/hydrogen/air mixtures (Figure 1.1(b)) across the tested mechanisms. For pure ammonia as fuel (Figure 1.1(a)), a substantial disparity is observed between the predictions of the different mechanisms. This disparity diminishes progressively with increasing hydrogen concentration in the fuel blend (Figure 1.1(b)), with the underlying cause under investigation.



(a) (b)

Figure 1.1: MFR experiments and simulations across kinetic mechanisms for (a) stoichiometric ammonia/air (inlet velocity 20 cm/s, max wall temperature 1430 K) and (b) stoichiometric 0.5 ammonia/0.5 hydrogen/air (30 cm/s, 1400 K), both at 1 atm. Mechanism differences are more evident in (a) than (b).

The core systems of the MFR, i.e., flow control and gas sampling at ultra-low flow rates, have been designed, assembled, and integrated, including gas cylinders, reactor-heating devices, and sampling/analytical systems. The GC-TCD and QMS were recommissioned (including TCD repair), and all tubing and sampling connections were completed, leak-tested, and secured. The MFR rig (see Figure 1.2) has entered final commissioning, with ongoing work on hydrogen quantification (GC-TCD), gas flow calibration, heating/temperature-measurement systems, and initial ammonia/hydrogen coflow tests. Once complete, the facility will enable well-controlled species measurements for validating ammonia/hydrogen kinetic models at low-to-intermediate temperatures.

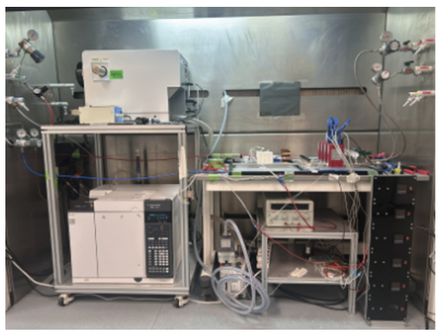


Figure 1.2: MFR rig in CARES lab with integrated gas-delivery, temperature-controlled reactor, GC-TCD, and QMS for species measurements during low-to-intermediate-temperature ammonia/hydrogen oxidation.

Development of detailed and reduced schemes

A systematic high-level ab initio study of hydrogen abstraction from N_2H_4 by ten combustion-relevant radicals was completed, determining electronic structures, reaction pathways, and temperature-dependent rate coefficients. Calculated rate coefficients were compared with literature data (see Figure 1.3), providing a consistent kinetic dataset for improving nitrogen-combustion mechanisms. A related conference paper has been submitted to the International Conference on Fluid Dynamics (ICFD 2026).

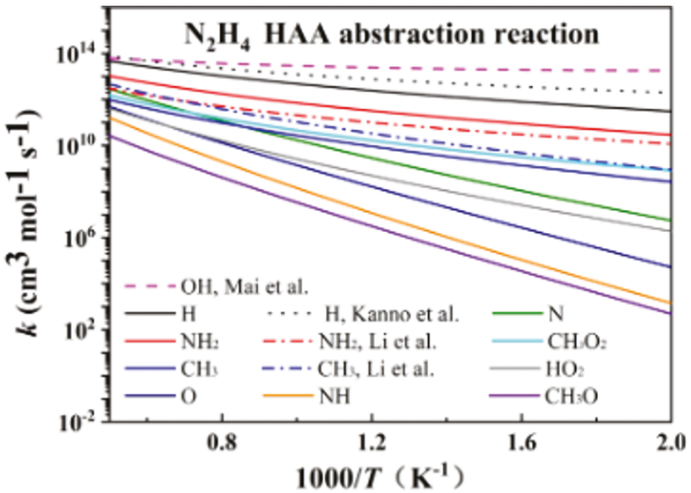


Figure 1.3: Arrhenius representation of the total rate constants for hydrogen abstraction from N_2H_4 by combustion-relevant radicals. Solid lines represent calculations from the present work, while dashed and dotted lines show available literature values. (Q.S. Li et al., J. Phys. Chem. A, 107, (2003), 6055-61; N. Kanno and T. Kito, Int. J. Chem. Kinet., 52, (2020), 548-55; T.V.-T. Mai et al., Phys. Chem. Chem. Phys., 21, (2019), 23733-41)

The framework was extended to hydrogen abstraction from cis- and trans-N_2H_2. Transition state searches, intrinsic reaction coordinate calculations, and Complete Active Space Second-Order Perturbation Theory (CASPT2) energy refinement have been completed for most trans- and several cis-N_2H_2 pathways. Current work focuses on reactant-complex optimisation and variational transition state treatment for selected low-barrier channels, followed by Master Equation System Solver (MESS) calculations of rate coefficients. A second conference paper on these N_2H_2 results was submitted to the 64th Symposium (Japanese) on Combustion, together providing new kinetic data for refining ammonia/hydrogen combustion mechanisms.

Literature kinetic mechanisms for partially cracked ammonia under partially premixed diffusion flame conditions (KAUST Flame D) were tested. All mechanisms showed similar behaviour with increasing strain rates, giving comparable extinction strain rates, with the main divergence in NOx predictions in the flame core, i.e., varying between detailed (40+ species, 250+ reactions) and light (~20 species, ~70 reactions) mechanisms. The (light and detailed) mechanisms were also compared against Tohoku University strain diffusion flame data. The light mechanisms were found to under-predict the extinction strain rate while the detailed mechanisms could not fully match experimental data across all conditions.

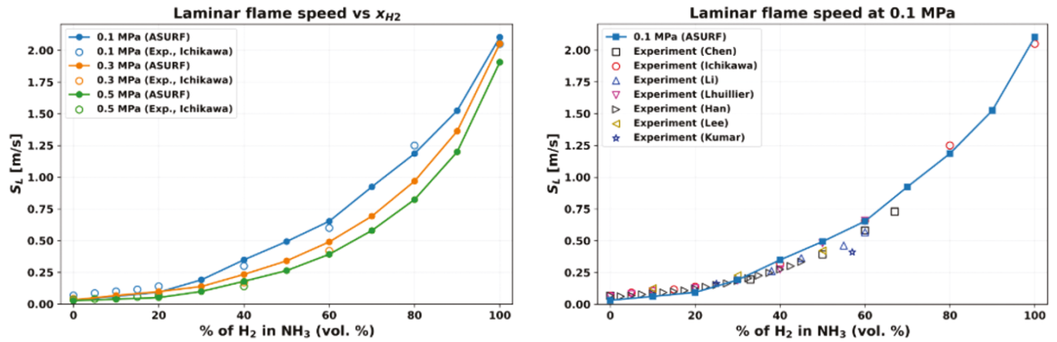
Additionally, a systematic numerical framework has been used to investigate the fundamental flame properties of ammonia/hydrogen mixtures. Using Cantera, freely propagating flame simulations were first performed to calculate laminar flame speeds over different hydrogen fractions and pressures of 1, 3, and 5 bar, with generally good agreement against available experimental measurements. In particular, the simulations at 3 and 5 bar extend the analysis beyond atmospheric conditions and provide a closer representation of the elevated-pressure environments encountered in practical combustors. This enables the pressure-dependent flame characteristics of ammonia/hydrogen mixtures to be assessed under conditions that are more relevant to real combustion systems and engineering applications.

The work was subsequently extended to counterflow premixed flames to investigate unstretched flame speed, flame stretch and Markstein length. A comprehensive sensitivity study was conducted using eight chemical kinetic mechanisms, different transport treatments (mixture-averaged, multicomponent and unity-Lewis-number), and the inclusion/exclusion of the hydrogen Soret effect. Their effects on laminar flame speed (S_L), Markstein length, flame thickness and combustion products were systematically evaluated.

Different methodologies for determining Markstein length and stretch-sensitive flame properties were also investigated, including the Egolfopoulos and Law approaches and local flame-based methods. This work has provided a more rigorous basis for understanding and modelling stretch and transport effects in ammonia/hydrogen premixed flames.

The ASURF simulation platform was successfully deployed on the National Supercomputing Centre (NSCC) Singapore, with the computational workflow being upgraded from serial to parallel computing for improved efficiency and scalability of large parametric calculations.

Systematic spherical flame simulations have subsequently been conducted at 1, 3 and 5 bar, covering eleven hydrogen fractions at each pressure (see Figure 1.4). These calculations are being used to investigate flame propagation, stretch effects, pressure dependence and flame stability, while establishing a numerical database for comparison with experimental measurements and higher-dimensional simulations.



(a) (b)

Figure 1.4: Comparison of ASURF-predicted laminar burning velocities using the POLIMI 2023 mechanism with experimental data. (a) pressure-dependent results and comparison with Ichikawa et al.; (b) results at 0.1 MPa and comparison with digitised experimental measurements.

WP2: FLAMES

Work Package 2 focuses on basic laminar and turbulent flames of increasing complexity, aiming to understand the effects of turbulence on the reaction zone and to assess novel flame stabilisation and ignition concepts relevant to gas turbines and reciprocating engines. In this reporting period, our progress includes the commissioning of new diagnostic systems, swirl-flame stability and lean blow-off measurements, and continued development of CMC-based modelling for partially cracked ammonia and hydrogen-enriched flames. Notably, the swirl-stabilised burner 'Swirl burner' is currently the burner used for performing collaborative research work with Siemens Energy.

Laminar hydrogen/ammonia/hydrocarbon flames

A laminar burner based on the design of Kagaya has been commissioned (see Figure 1.5(a)), including a chiller that supplies cooling water to maintain a controlled, fixed wall temperature. The gas supply manifold and piping were fabricated and installed to enable delivery of air and multiple fuel types. In addition, a tuneable diode laser absorption spectroscopy (TDLAS) system has been installed to perform line-of-sight measurements of temperature and H_2O concentration. Several preliminary experiments were conducted on the burner using methane flames to measure temperature and H_2O concentration (see Figure 1.5(b)). The next step is to validate the laser-based measurements against reference diagnostics, namely a known flame condition for H_2O mole fraction retrieval and a thermocouple measurement for temperature.

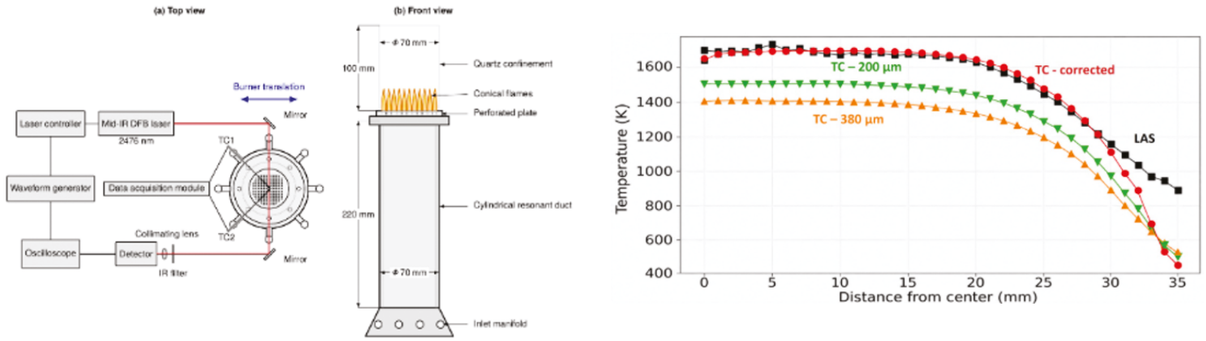


Figure 1.5: (a) Schematic of the experimental setup for TDLAS system. (b) Temperature profile of the hydrogen/ammonia flame validation experiment (TDLAS versus thermocouples).

A laminar coflow diffusion flame burner has also been commissioned, and soot formation studies have been performed using this setup (see Figure 1.6). Ethylene was blended with ammonia at varying degrees of cracking (i.e., non-cracked (A0), partially cracked (A25, A50, A75), and fully cracked (A100)) to observe the resulting effect on soot formation. Blending with non-cracked ammonia was found to reduce the soot volume fraction signal, while fully cracked ammonia (i.e., its hydrogen and nitrogen decomposition products) increased it. Partially cracked ammonia gave intermediate results, scaling with how close the blend was to fully cracked or non-cracked composition.

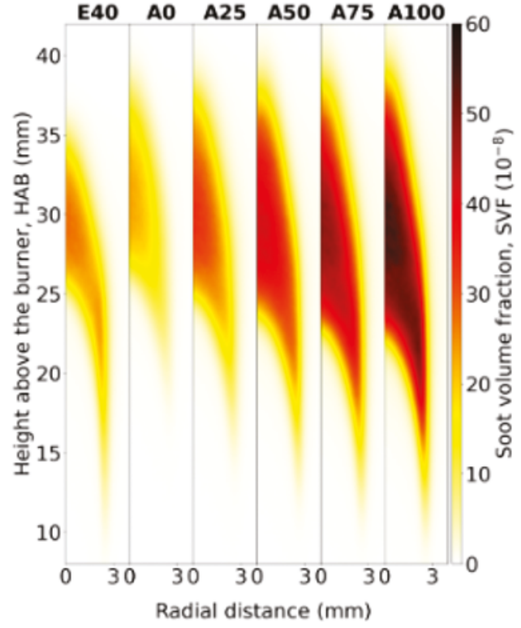


Figure 1.6: Soot volume fraction profiles of laminar coflow ethylene flames blended with ammonia at varying degrees of cracking.

Experiments with turbulent ammonia/hydrogen swirl flames

Non-premixed ammonia/hydrogen flames were studied using a Swirl-stabilised burner 'Swirl burner', with lean blow-off (LBO) limits measured across a range of ammonia volume fractions and bulk velocities. Flame structures under both axial and radial fuel injection were captured and compared at fixed power but varying ammonia volume fractions, using OH-PLIF and OH*/NH_2* chemiluminescence diagnostics (see Figure 1.7). Axial non-premixed ammonia flames were further investigated under conditions approaching LBO, including the effect of secondary air injection on both blow-off limits and flame structure. Ongoing research work with Siemens Energy using this Swirl burner is now focused on testing a new ammonia combustion concept, developed in collaboration with Siemens Energy researchers.

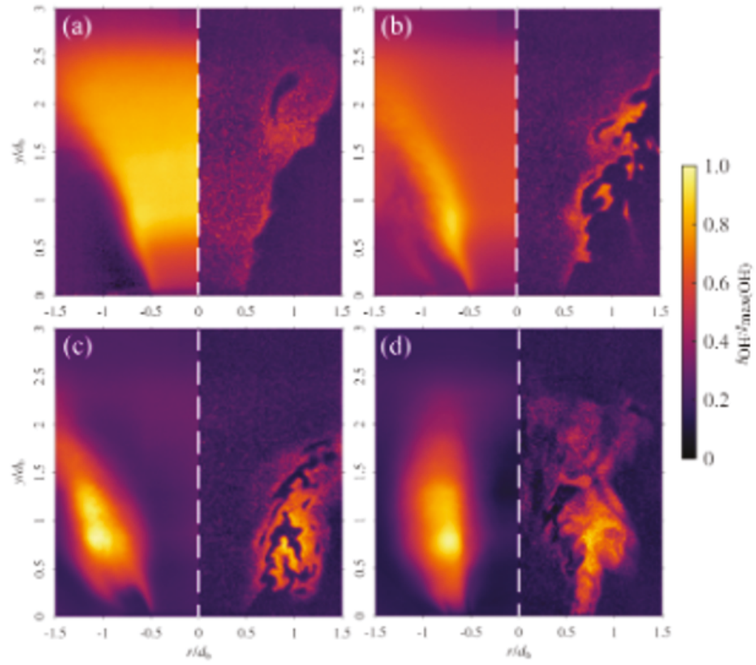


Figure 1.7: Normalised, averaged and instantaneous OH-PLIF images of radial-injected non-premixed ammonia/hydrogen/nitrogen flames at various ammonia volume fractions. (a) 100% ammonia; (b) ammonia/hydrogen/nitrogen = 70%/22.5%/7.5%; (c) ammonia/hydrogen/nitrogen = 40%/45%/15%; (d) ammonia/hydrogen/nitrogen = 10%/67.5%/22.5%.

In parallel, premixed methane flames with premixed and non-premixed hydrogen injection were studied using OH-PLIF and OH*/CH* chemiluminescence imaging, to better understand how hydrogen addition and injection mode affect flame structure. This work, together with earlier results on the same configuration, has been incorporated into a manuscript now being prepared for journal submission.

We have also furthered our understanding on the structure and stability of lean premixed swirl flames (using the Swirl burner) fuelled by methane and hydrogen-enriched methane, with relevance to low-carbon gas turbine combustion. Experiments were performed in the Swirl burner (premixed) to examine how hydrogen enrichment and swirl intensity influence flame morphology and heat release distribution, using OH* chemiluminescence diagnostics. The results show that hydrogen addition significantly modifies flame structure under lean conditions (i.e., equivalence ratio 0.8). Compared with pure methane, hydrogen-enriched flames exhibit a more compact and spatially concentrated high-OH region, indicating enhanced reactivity and localised heat release (Figure 1.8). These changes are associated with improved flame anchoring and stabilisation in the swirl-stabilised flow, highlighting the potential of hydrogen blending to extend lean operability while maintaining stable combustion.

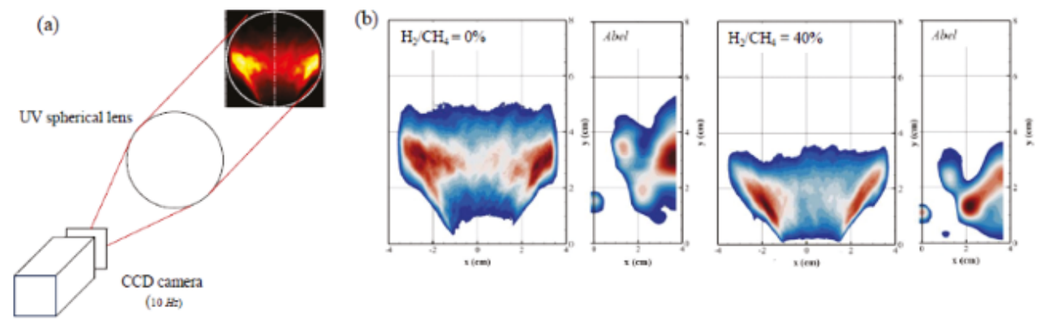


Figure 1.8: (a) Schematic of the chemiluminescence setup used to infer the time-resolved flame shape. (b) Averaged OH chemiluminescence normalised to the maximum value (I_{OH}/I_{max}) and their inverse Abel transform for each case illustrating the effect of the percentages of hydrogen addition to methane flame on the OH chemiluminescence at equivalence ratio 0.8.*

Spark ignition and plasma-assisted stabilisation

Ammonia/air flames are difficult to ignite due to their narrow range of ignitable conditions, which is a key challenge in the development of gas turbines fuelled by ammonia. One of the major challenges that needs to be addressed is achieving reliable ignition in ammonia gas turbines. Hence, the Swirl burner, along with a laser ignition were used to investigate flame ignition methods for ammonia-fuelled gas turbines. Ignition was achieved using a focused Nd:YAG laser (1064 nm) as the ignition source. For both premixed and non-premixed ammonia/air flames, an ignition probability map was built for each equivalence ratio (see Figure 1.9 for setup). The ignition probability map allows the identification of favourable ignition locations inside the combustor across different equivalence ratios, informing ignition strategy for ammonia-fuelled gas turbines.

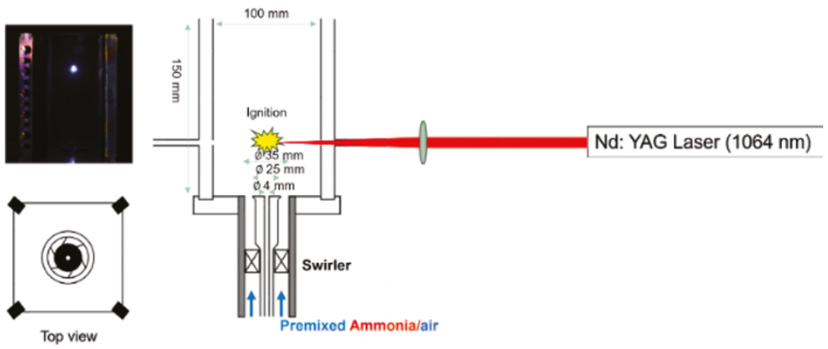


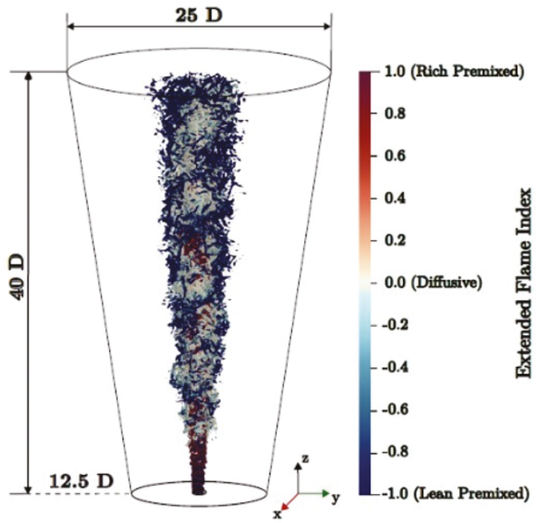
Figure 1.9: Schematic of the swirl burner and laser ignition setup, with a top-view of the swirler and a photograph of a laser-ignited flame kernel (inset). The premixed ammonia/air mixture enters through the swirler, and the focused Nd:YAG laser beam (1064 nm) is directed through a convex lens to the ignition location.

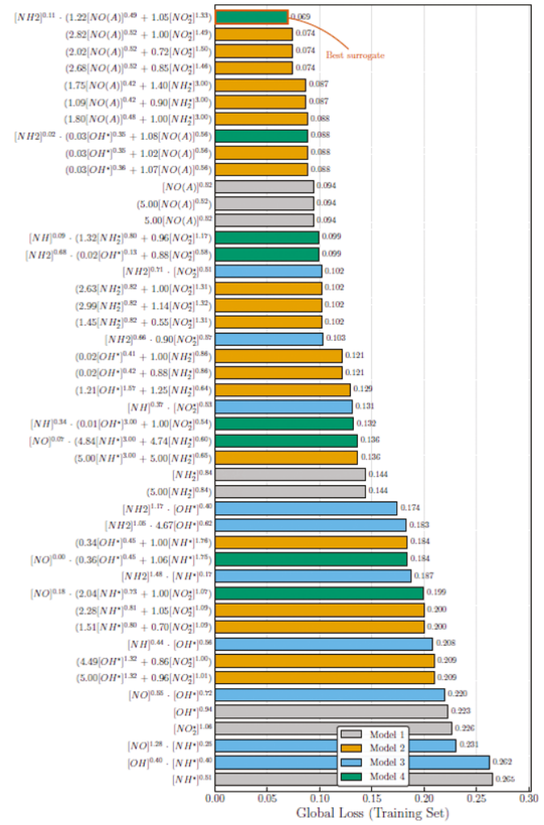
Modelling ammonia/hydrogen turbulent flames

We have made progress in the development of numerical solver, analysis of fuel-flexible flames, large-eddy simulation of ammonia jet flames, and post-processing of DNS (Direct Numerical Simulation).

In the development of numerical solver, a 0D-CMC solver (built around the G-Scheme reduced-chemistry integrator to make detailed chemistry affordable inside large simulations) was completed and validated. The solver now matches with the reference to within three degrees in peak flame temperature across every test case (hydrogen and methane fuels, small and detailed mechanisms, ignition and steady flamelet conditions), with no integration failures. An optimisation campaign in June 2026, including a new analytic Jacobian, made the integrator 1.2 to 2.7 times faster than the reference on flamelet cases and around eight times faster than a conventional implicit baseline on detailed methane chemistry; two stability defects introduced by the optimisation were traced and fixed, and the code now passes its full regression suite. This solver is the piece that directly enables the LES-CMC simulations planned in HYCOMBS. In parallel, and in collaboration with Sapienza University of Rome, an explicit solver was integrated into the 0D-CMC code to accelerate the chemical kinetics calculation (typically the most computationally expensive part of the simulation) with the implementation tested for stability and performance; if validated, this will further reduce CPU time and allow more complex chemical mechanisms in practical engineering applications.

On fuel-flexible flames, a manuscript titled "Evaluation of Heat Release Rate Markers for Partially Cracked Ammonia Combustion with Air" has been submitted and is now under review at *Combustion Science and Technology*. Since heat release cannot be measured directly in a flame, and the optical markers that work for conventional fuels fail for ammonia, the study turned to high-fidelity simulation data of a partially cracked ammonia jet flame, capturing lean-premixed, non-premixed, and rich-premixed combustion modes across the turbulent flame brush (Figure 1.10 (a)). Screening candidate marker formulations against this dataset identified a pair of nitrogen-oxide based signals that reliably track heat release across all three regimes (Figure 1.10 (b)). This gives combustor developers a physically grounded diagnostic target.





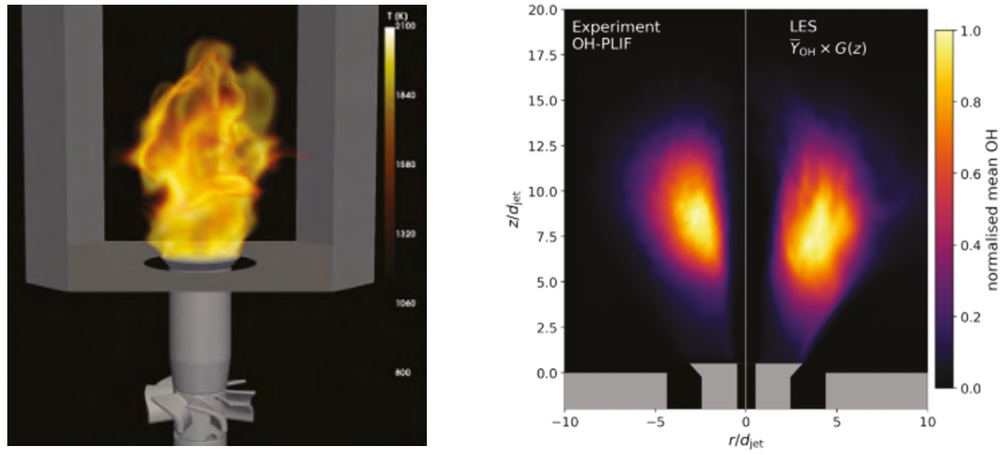
(a) (b)

Figure 1.10: (a) Computational domain showing the instantaneous Extended Flame Index (FI) field conditioned to the active reaction zone (HRR > 0.01·HRR_{max}). Positive Q-criterion iso-surfaces highlight the turbulent vortical structures, while the FI delineates lean-premixed (≈ −1), non-premixed (≈ 0), and rich-premixed (≈ 1) combustion modes. (b) Global training loss ϵ_{global} for all screened surrogate formulations, grouped by architecture class (single-species, multiplicative pair, additive dual-excited, and hybrid multiplicative-additive). The hybrid additive form anchored on NH_2 attains the lowest loss (0.069), narrowly ahead of the anchor-free additive pair NO(A) + NO_2^* (0.074). Fitted anchor exponents are uniformly small, and several hybrid forms collapse onto their anchor-free counterparts.

The large-eddy simulation (LES) work centred on the KAUST jet flame and the Swirl burner. For the KAUST flame, work is moving towards a-posteriori simulations, building on and validating what the a-priori analysis of the Tohoku DNS data had already suggested about preferential and differential diffusion modelling in high-hydrogen-content mixtures. For the Swirl burner, mesh quality was refined by improving grid topology and orthogonality, enabling higher-order numerical schemes while maintaining computational stability; reverse-engineering the swirler geometry and remeshing on this basis resolved the convergence problems and mismatches previously seen, and is fundamental to capturing complex flow-flame interactions accurately. This work was presented as a poster at the World Hydrogen Energy Conference (WHEC 2026).

A comprehensive post-processing study was also initiated on a DNS dataset of a turbulent jet flame (KAUST Flame D), focusing on sub-grid modelling (differential and preferential diffusion terms within the LES equations, including filtered mixture fraction, progress variable, their respective variances, and enthalpy) and reaction zone identification, evaluating chemical markers (excited species) to identify reaction zones in both premixed and non-premixed combustion regimes.

Separately, work continues on improving the differential diffusion effect in the CMC framework to achieve closer agreement between LES simulations and the experimental results of the KAUST Flame F. LES simulation of the Swirl burner experiment recently performed for a partially cracked ammonia swirl flame in the Swirl burner has also begun (see Figure 1.11). The early results, using simple models with some phenomena still missing, are already able to predict flame height, and these simulations will subsequently feed into lower-order models to explore a wider range of operating conditions.



(a) (b)

Figure 1.11: (a) 3D visualisation of the instantaneous temperature field obtained from the LES simulation (b) Comparison of the experimental mean OH-PLIF signal against the mean OH from the LES simulation for a jet fuel blend composed of 70% ammonia, 22.5% hydrogen, and 7.5% nitrogen.

WP3: NOVEL COMBUSTION SYSTEMS FOR GAS TURBINES

Work Package 3 aims to investigate the structure of gas turbine combustion of hydrogen and ammonia, using high-flow-rate and high-pressure experiments to generate knowledge and data closer to practical application. The progress in the current reporting period includes manufacturing and commissioning of a new staged combustion rig, upgrades to supporting laser-diagnostic infrastructure, and continued dissemination of thermoacoustic findings at international conferences.

Design of a new experimental combustion setup has progressed from detailed design drawings into manufacturing. The rig will be capable of staged operation and independent acoustic excitation of primary and secondary stages. Metal 3D-printed components have been produced, aluminium machined parts have been ordered, and the remaining steel parts have been requested from the NUS Central Workshop and are awaiting a quotation. Key equipment, including microphones, amplifiers, MFCs, DAQs, PMTs, cameras, and PIV systems, has been received and integrated into the CARES lab, and the acoustic forcing system has been specified and ordered. Work in the coming reporting period will focus on assembling the new setup, followed by acoustic characterisation of all rig elements to support accurate acoustic modelling and to verify and quantify the controlled injector acoustic impedances.

Research output from this work package has been presented at two conferences. At WHEC 2026 in Singapore, some of the first experimental HYCOMBS thermoacoustics results, focusing on acoustic characterisation of the new setup and its ability to vary inlet impedance (see Figure 1.12) have been presented. At the International Symposium on Combustion in Kyoto, an oral presentation based on previously obtained data from an axially staged system exhibiting self-excited thermoacoustic instabilities, analysing the timescales of heat release rate oscillations in both primary and secondary stages and how these can be manipulated to suppress instability. The work has also been accepted for publication.

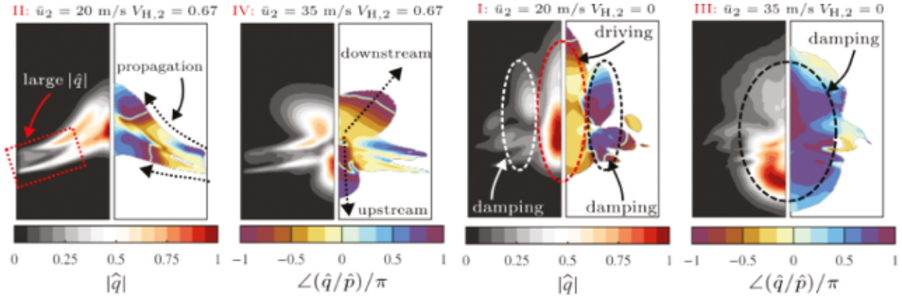


Figure 1.12: Normalised heat release rate fluctuation magnitude $|\hat{q}|$ and phase angle $\angle(\hat{q}/\hat{p})/\pi$ relative to the local pressure fluctuation, for four operating conditions spanning bulk velocity ($\bar{u}_2$ = 20 and 35 m/s) and hydrogen volume fraction ($V_{H,2}$ = 0 and 0.67). Regions of driving and damping are identified from the phase relationship between heat release and pressure, with Case II additionally showing evidence of downstream/upstream disturbance propagation.

WP4: NOVEL COMBUSTION SYSTEMS FOR RECIPROCATING ENGINES

Work Package 4 focuses on the investigation of combustion systems for reciprocating engines, where the difference in the combustion chamber volume and wall effects can affect the ignition behaviour and pollutant formation differently than in gas turbines. In the current reporting period, we have focused on advanced ignition and combustion of ammonia blend fuels, combining experimental and numerical studies to support the development of ammonia-fuelled internal combustion engines. This includes commissioning of the constant volume combustion chamber (CVCC) and physics-based analysis of knocking behaviour in spark-ignition (SI) engines.

Ammonia/hydrogen and hydrocarbons/ammonia flame structure in high-pressure CVCC

The control, fuel supply, ignition, and diagnostic systems of the CVCC have been fully installed and commissioned. The facility is currently awaiting approval from the National Environment Agency (NEA) for the ammonia-use permit and final internal safety approval for the hydrogen control panel following completion of the relevant requirements from the Singapore Civil Defence Force (SCDF). Once these approvals are obtained, the upgraded facility will be ready for subsequent ammonia/hydrogen combustion experiments. In parallel, preliminary analysis of the previously acquired passive pre-chamber ignition data has been conducted. Representative flame image in the CVCC and chamber-pressure histories are shown in Figure 1.13(a) and 1.13(b), respectively.

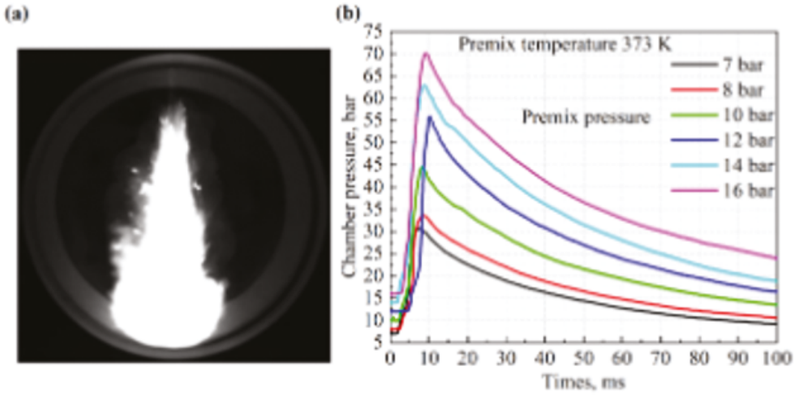


Figure 1.13: (a) Passive pre-chamber ignition with premixed hydrogen/ammonia (b) CVCC chamber pressure history at different pressures.

As shown in Figure 1.13(b), a rapid pressure rise was observed following ignition, followed by a gradual pressure decay as the combustion process evolved. Increasing the initial premix pressure from 7 bar to 16 bar significantly increased the peak chamber pressure, from 30 bar to nearly 70 bar, while the overall pressure evolution characteristics remained similar. These results demonstrate the strong influence of the initial charge pressure on combustion intensity and provide an initial basis for evaluating the ignition and combustion characteristics of the passive pre-chamber system.

Predicting knock onset in ammonia/hydrogen-fuelled spark ignition engines

Hydrogen addition, combined with the high temperature and pressure conditions associated with high-compression-ratio engines, raises important questions regarding the knock propensity of ammonia/hydrogen-fuelled engines. The fundamental mechanisms governing knock initiation and development in ammonia combustion remain only partially understood. Hence, the team from the University of Orléans, in collaboration with the Tohoku University team have applied a combined experimental and numerical approach to predict the temperature and pressure conditions at knock onset in a SI engine with a compression ratio of 16.4, fuelled with ammonia/10% hydrogen. Constant-volume 1D DNS simulations were performed using the COGNAC code developed at Tohoku University and previously validated for hydrocarbon fuels, enabling flame autoignition interactions to be resolved at the microscale. A two-zone model (2ZM), implemented in ANSYS Chemkin-PRO and based on experimental data obtained at the University of Orléans, was used to track the evolution of the unburnt-gas volume, particularly near knock onset.

As shown in Figure 1.14(c), the 1D DNS simulations successfully reproduced the physical transition toward knock (see the transition from '+' to '×' to '◆' in Figure 14(c)), which was not captured by the 2ZM (see Figure 1.14(b)). Nevertheless, both approaches predicted very similar pressure and temperature conditions at knock onset '×' and consistently captured the evolution of chemical species through three characteristic stages: initialisation, pre-knock, and knock. The 1D DNS analysis further highlighted the role of H_2O_2 decomposition, providing new insight into the chemical pathways associated with ammonia decomposition and the transition toward autoignition.

Additionally, a novel and unexpected connection between a macroscopic theoretical framework and detailed numerical predictions of knock onset was reported. Knocking conditions in SI engines was successfully predicted based on the mode transition between two flame propagation regimes, i.e., Zel'dovich–Frank-Kamenetskii (ZFK) mode to the Fisher-Kolmogorov-Petrovsky-Piskunov (FKPP) mode. Despite this physics-based simple analysis is coarse (i.e., macroscopic framework that does not resolve fine-scale details), the transition conditions computed using detailed chemical reaction mechanisms for the specific target mixtures are consistent with the knock onset obtained from the DNS. This remarkable agreement demonstrates that, by numerically analysing the ZFK–FKPP transition with realistic chemistry for a given mixture, the DNS knock onset can be predicted.

The work provides a valuable framework for understanding and predicting knock onset in ammonia/hydrogen-fuelled engines. Beyond improving the fundamental understanding of ammonia combustion, this approach can support the optimisation of future zero-carbon powertrain and genset technologies through appropriate hydrogen blending. Within the HYCOMBS project, the methodology will subsequently be extended to ammonia/hydrogen mixtures with higher hydrogen contents, for which increased reactivity is expected to promote more severe knock phenomena.

Engine combustion and emissions modelling

In addition to the DNS work above, complementary numerical studies were conducted at both engine and spray combustion. For an ammonia/natural gas/diesel marine engine, a validated 3D CFD model was used to evaluate diesel injection strategies. Pilot/main injection coordinated reactivity stratification with near TDC activation, improving thermal efficiency and substantially reducing ammonia/methane slip and greenhouse gas emissions, although with a NOx trade off (see Figures 1.16(a) and 1.16(b)). A second CFD study examined n-heptane-piloted liquid-ammonia cross-spray combustion in the CVCC. The results show that injection phasing governs the thermochemical overlap between pilot oxidation and ammonia activation, which determines whether sustained main heat release can be established (see Figures 1.16(c) and 1.16(d)).

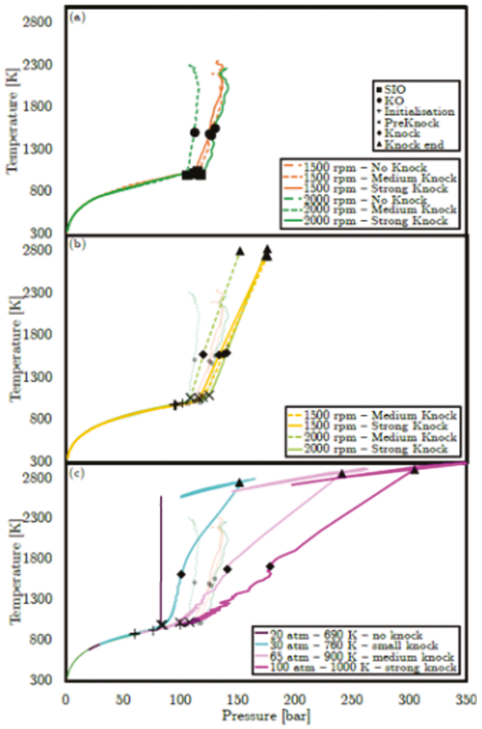


Figure 1.14: Temperature-Pressure evolution for the experiment and both numerical methods. Each figure highlights either (a) Experiment, (b) 0D 2ZM, or (c)1D DNS.

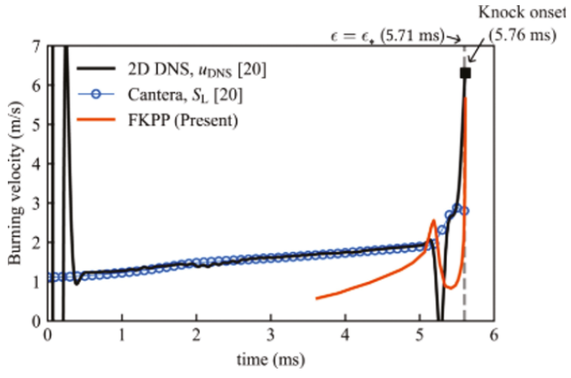


Figure 1.15: Comparison of instantaneous burning velocities obtained from 2D DNS (black curve), Cantera simulation (blue curve), and FKPP formula (red curve). The dashed line represents critical timing (t_*) where $\epsilon = \epsilon_*$ (5.71 ms), and the closed square indicates the knock onset (5.76 ms).

The above research outcomes have also been disseminated through international conferences. Related work was selected for oral presentation at WHEC 2026, and The International Symposium on Thermal-Fluid Dynamics (ISTFD), with the work presented at ISTFD receiving the Best Paper Award. In addition, the two numerical studies described above are progressing toward journal publication: one manuscript has been submitted to *Fuel* and is currently under review, while the other has been completed and is undergoing final revision prior to submission.

Collaborative Research on Optical-Engine Combustion

Alongside this fundamental ammonia/hydrogen simulation work, we have collaborated with researchers from Tohoku University and Shanghai Jiao Tong University on the analysis of knocking combustion data. This work involved high-speed natural flame luminosity imaging, POD analysis, Hovmöller analysis, and optical-flow-based approaches to investigate combustion instability, auto-ignition, and knock-induced wave/flow structures. These complement the fundamental flame research above and broadening the application of advanced combustion-data analysis techniques.

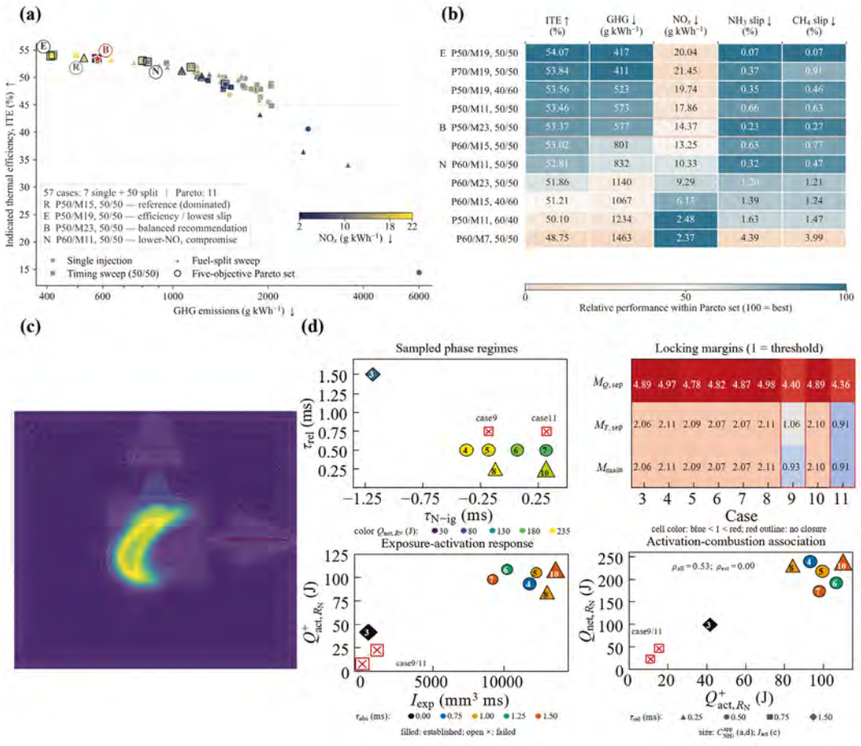


Figure 1.16: Multi-objective assessment and combustion analysis of the investigated injection strategies. (a) ITE–GHG trade-offs for the 57 cases. (b) Relative performance of the Pareto-optimal cases. (c) Mesh-refinement strategy with fixed near-nozzle refinement and gradient-based adaptive refinement. (d) Representative combustion regimes and exposure-activation-combustion relationships for the diesel/ammonia/diesel cases.

WP5: DEPLOYMENT

Work Package 5 focuses on the translation of the fundamental science produced across the WPs 1 to 4, so as to enable them to be ready to be deployed by the industry and undergo technological transfer to the industry. The progress in the current reporting period includes high-fidelity simulations of detonation inhibition and detonation-vortex interactions, techno-economic and low-order combustion modelling for industrial decarbonisation applications and continued academic dissemination of these results.

Design tools for industry

We developed a conceptual design for an integrated steam methane reforming and carbon capture system (SMR-H2), for hydrogen-fuelled marine gas turbine systems. The design incorporates hydrogen production, pre-combustion CO_2 capture, waste-heat recovery, and onboard LNG and captured-CO_2 storage within the reference bulk carrier, considering its space constraints (Figure 1.17). The vessel particulars and operational data were provided by our industry partners, Laskaridis Shipping Co. Ltd. and METIS Cyberspace Technology. Subsequent work investigated combined-cycle gas turbine (CCGT) architectures integrated with pre-CCS, showing that onboard blue hydrogen production efficiency can be further improved through combined-cycle power generation.

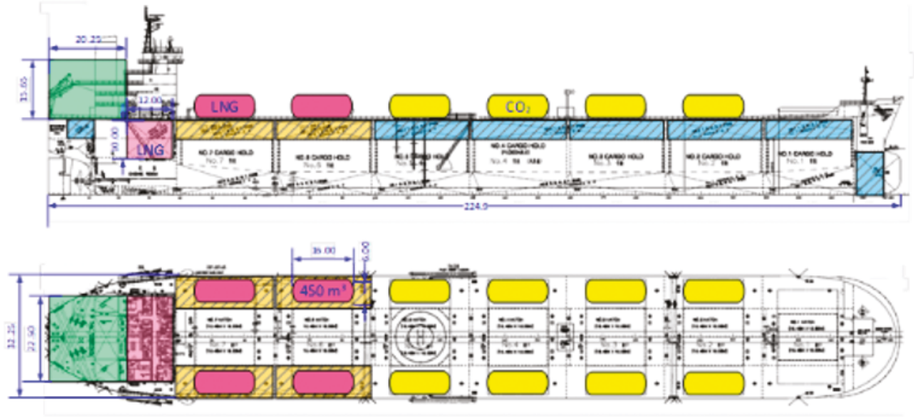


Figure 1.17: The general arrangement for the reference ship retrofitted with onboard hydrogen production and pre-combustion carbon capture system (PreCCS). A total of 12 Type C cylindrical storage tanks (approximately 450 m^3 each; radius 3 m, length 16 m) are installed symmetrically along the port and starboard sides. These include 4 tanks for storage of LNG fuel and 8 tanks for captured CO_2. The red-shaded volume represents the reserved space for the LNG storage tank (approximately 2,700 m^3), while the green-shaded volume indicates the allocated space for the PreCCS plant. The layout utilises available deck space and aft sections to accommodate additional equipment, enabling system integration without compromising cargo hold capacity.

A techno-economic assessment was then conducted to compare the technical, environmental, and economic performance of SMR-H_2 with other low-carbon pathways, including green hydrogen, ammonia, methanol, biodiesel, and post-combustion carbon capture. The assessment considered capital and operating costs, fuel consumption, emissions reduction, revenue losses arising from reduced cargo capacity, and the effects of emerging maritime regulations and penalties. The results show that producing hydrogen onboard can be more cost effective than bunkering green hydrogen or other green fuels such as ammonia and methanol, whose prices are strongly influenced by the high cost of renewable electricity, provided the energy penalty remains low and a high CO_2 reduction rate can be achieved. The SMR-H_2 pathway thus offers a lower CO_2 abatement cost than most alternative-fuel options, with abatement costs that remain comparatively stable under different fuel-price and regulatory-policy scenarios. This indicates greater economic resilience and a potentially more predictable decarbonisation pathway for shipowners (see Figure 1.18).

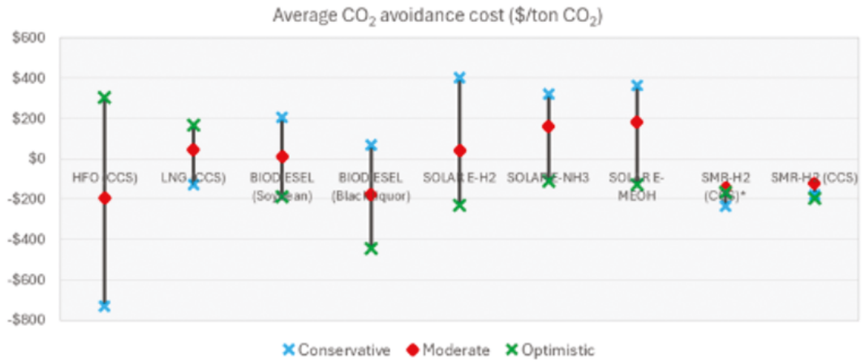


Figure 1.18: The average CO_2 avoidance cost of various low-carbon pathways under conservative, moderate and optimistic scenarios.

Two papers have been prepared based on this work, covering the conceptual design and techno-economic assessment of low-carbon retrofit pathways for bulk carriers; the proposed data-driven decarbonisation strategy could also be adapted for other ship types and relevant land-based applications. As a next step, laboratory experiments will combust reformate (the hydrogen-rich gas from pre-CCS) blended with methane (0–100%) to characterise emissions (CO, CO_2, NOx) as a function of fuel composition. These results will develop and validate a reactor network combustion model to simulate gas turbine emissions under varying fuel blends and operating conditions, ultimately integrated with the pre-CCS/CCGT financial model for techno-economic optimisation.

In parallel, a financial model for onboard hydrogen production has been developed and coupled with a stochastic framework to evaluate financial and investment risks for hydrogen-enabled vessels under uncertainties in fuel prices, emissions surplus rewards, and carbon pricing penalties. This is a business model intended to apply to the maritime sector, including the Singapore context, and to support projections of energy use within the sector. Additional research activities include biofuel route planning and optimisation for low-carbon vessel operations, and Laser-Induced Breakdown Spectroscopy testing to determine biofuel origin and authenticity.

Detonation

Hydrogen's low ignition energy and high flammability pose explosion risks that limits its widespread adoption. Here, we have conducted high-fidelity simulations of hydrogen-air detonation initiation with detailed chemistry (37 species and 174 reactions), and the mixture is premixed with a chemical inhibitor, i.e., trifluoroiodomethane (CF_3I). As shown in Figure 1.19(a), without CF_3I the detonation propagates radially with the shock and reaction zone tightly coupled in the hydrogen-air detonation initiation. By adding the inhibitor, Figures 1.19(b) and 1.19(c) show that the shock and reaction zone decouples firstly at the diagonal direction, and then the decoupling region propagates circumferentially to the x and y axes. Such a decoupling transits the detonation to a shock wave with much weaker strength and is potentially effective to reduce the damage caused by hydrogen detonations in practical applications. The progress of the study was presented at the International Symposium on Combustion in Kyoto.

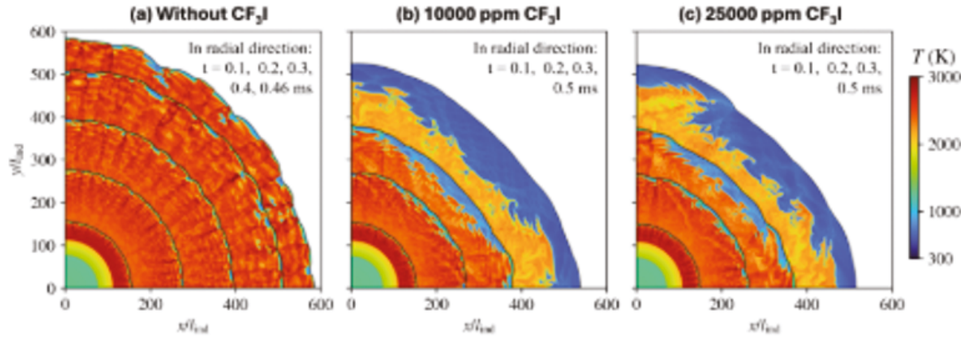


Figure 1.19: Hydrogen-air detonation propagation (a) without CF_3I; (b) with 10,000 ppm of CF_3I; (c) with 25,000 ppm of CF_3I.

To support large-scale detonation simulation with detailed chemistry, a dynamic load-balance algorithm is developed to distribute the chemistry computation workloads among different cores/nodes on-the-fly. This algorithm, combined with a previously developed GPU-CPU hybrid detonation solver, makes the simulation more efficient. Moreover, the solver was applied to simulate 3D hydrogen detonation. Figure 1.20 presents the numerical soot foil (i.e., peak-pressure record in each grid) of such a simulation. It is plotted based on a physical time of 0.06 ms, which takes 8.35 hours for computation using 256 CPU cores and 16 Nvidia A100 GPUs, with only 2.2 hours for chemistry integration due to GPU acceleration. The results are presented as a poster at the National Supercomputing Centre (NSCC) ASPIRE2B launch event in Singapore. The progress creates a solid foundation for larger-scale simulations in future work.

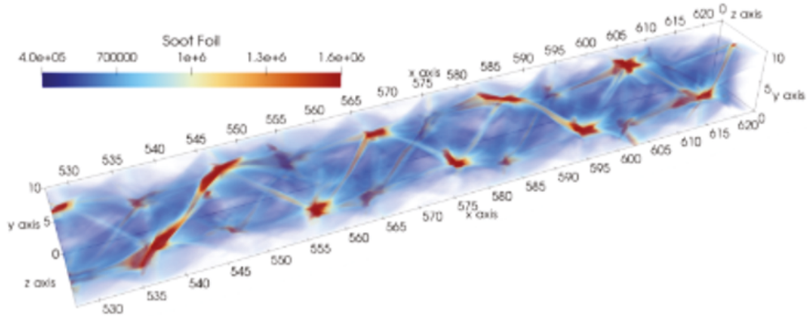


Figure 1.20: Numerical soot foil distribution from large-scale detonation simulation.

Additionally, significant progress has been made in the numerical investigation of detonation–vortex interactions, with the objective of improving the fundamental understanding of detonation propagation in vortical flow environments relevant to advanced propulsion systems. The study focuses on the interaction between a gaseous detonation wave and an isolated Gaussian vortex using high-resolution numerical simulations with detailed hydrogen chemical kinetics. The numerical framework has been established using the GPU-accelerated PeleC solver with adaptive mesh refinement.

The simulations demonstrate that the vortex introduces non-uniform incoming-flow velocity perturbations, which locally modify the detonation propagation velocity and produce pronounced deformation of the

wave front (see Figure 1.21). This deformation alters triple-point trajectories and stretches the cellular structure before the detonation gradually recovers downstream. Further analysis shows that increased front curvature enhances the misalignment between pressure and density gradients, thereby strengthening baroclinic vorticity generation. Quantitatively, the mean vorticity magnitude increases by approximately 14.9% following the interaction. Validation against published numerical and experimental data, together with a grid-independence study, has confirmed that the computational approach can reliably resolve the cellular detonation structure and reaction zone.

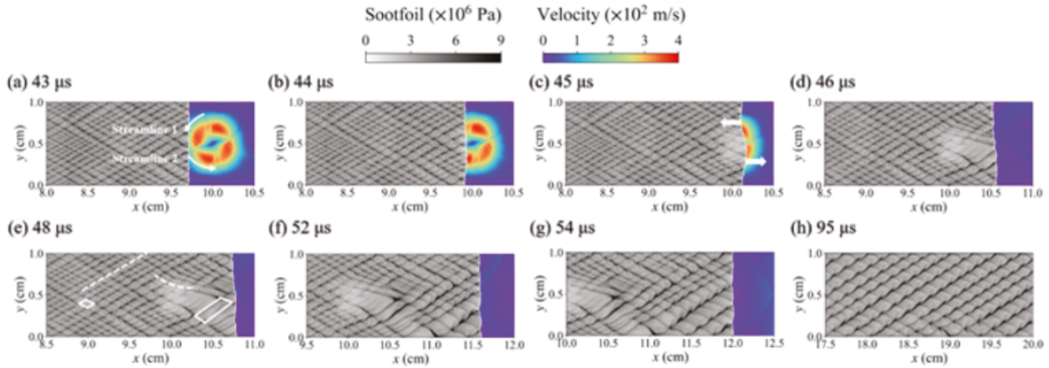


Figure 1.21: Flow field evolution during the detonation–vortex interaction.

The influence of the vortex on chemical reactions has also been quantified. The vortex-induced deformation weakens the local post-shock thermodynamic state, delays ignition, and increases the amount of residual unburned hydrogen. Statistical analysis indicates that the mean induction-zone length increases from 141.6 μm to 205.0 μm, corresponding to an increase of 44.8%, demonstrating a substantial delay in chemical energy release over a large portion of the detonation front. A parametric study has additionally been conducted to examine the effects of vortex strength, vortex radius, and mixture composition. The results indicate that vortex strength and radius are the dominant parameters controlling front deformation, whereas mixture composition mainly modifies the intrinsic cellular structure and has a comparatively weaker influence on the overall deformation.

Overall, the current work establishes a clear physical link between vortex-induced velocity perturbations, detonation-front deformation, enhanced vorticity generation, and delayed chemical reactions. A manuscript titled "Numerical investigation of detonation interaction with an isolated vortex" has been prepared based on these results. The next stage will extend the present framework toward more realistic vortical and turbulent environments, including 3D configurations, to further assess detonation dynamics under conditions relevant to practical propulsion systems.

Effects of azimuthal mode number on a reactive hydrogen bubble impacted by a convergent shock

Shock-driven instabilities in converging geometries play a critical role in inertial confinement fusion, and scramjet combustion. Richtmyer–Meshkov (RM) instability, in which a perturbed interface between fluids of different densities is impulsively accelerated by a shock wave, evolves from linear growth into nonlinear development and ultimately turbulent mixing. While the phenomenon is well studied in its inert form, the combined effects of chemical reactions and azimuthal mode number on reactive double-layer gas cylinders under convergent shocks remain insufficiently understood. To address this, 2D direct numerical simulations of a cylindrical RM instability were performed, with and without chemical reactions, to clarify how azimuthal mode number governs shock focusing, instability growth, and detonation initiation in a double-layer hydrogen gas cylinder. The results show that increasing the azimuthal mode number significantly modifies interface geometry and strengthens shock focusing, leading to the formation of a reflected transmitted shock (RTS). The jet head behind the RTS propagates outward, deforming the inner interface and generating outward-directed jets in the spike regions (Figure 1.22).

Interaction between the transmitted shock and the perturbed inner interface deposits substantial baroclinic vorticity at higher mode numbers, accelerating the growth of RM instability on the bubble side; higher mode numbers also generate more transverse waves and reflections, introducing stronger pressure perturbations and additional vorticity along interfaces and slip lines, and so further enhancing interfacial deformation and mixing ahead of ignition. Notably, the inert cases show stronger instability growth and higher interfacial mixing fractions at both interfaces than the reactive cases.

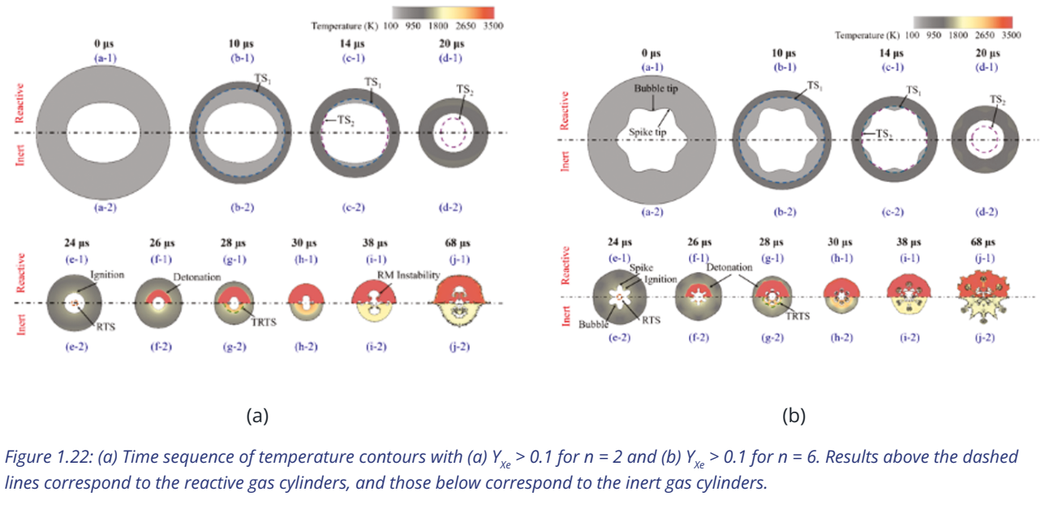


Figure 1.22: (a) Time sequence of temperature contours with (a) $Y_{Xe} > 0.1$ for n = 2 and (b) $Y_{Xe} > 0.1$ for n = 6. Results above the dashed lines correspond to the reactive gas cylinders, and those below correspond to the inert gas cylinders.

Hotspots originate from localised compression induced by transverse-wave interactions after shock focusing, elevating temperature and pressure in the spike regions and triggering ignition, followed by an outward-propagating detonation wave. Once this detonation reaches the outer interface, the reflected rarefaction wave interacts with the inner interface, inducing Rayleigh–Taylor instability and further amplifying deformation and mixing at higher mode numbers. Thermal decomposition behind the outward-propagating RTS subsequently reduces the total heat release rate. Chemical explosive mode analysis (CEMA) further shows that ignition evolves from radical-driven chain branching to thermal runaway. Together, these results clarify the coupling between hydrodynamic instability and reactive-wave dynamics in convergent geometries, with implications for predicting ignition timing, detonation onset, and mixing efficiency in combustion and propulsion systems. A manuscript based on this work has been submitted to *Fuel*, and an abstract has been submitted to the WHEC 2026. The next step is to complete the CEMA analysis to identify the dominant species and elementary reactions responsible for chemical ignition, and to articulate the detailed ignition mechanism.

Industrial visit

HYCOMBS hosted a technical tour for Siemens Energy at our CARES lab facilities, providing an opportunity for detailed exchange on our combustion research capabilities and decarbonisation technologies. The visit facilitated in-depth discussions between our researchers and the Siemens Energy delegation on challenges and opportunities in hydrogen and ammonia combustion for power generation applications. The engagement strengthened ongoing collaboration between HYCOMBS Research Fellows and Siemens Energy research scientists, establishing a direct pathway for translating lab innovations into industrial gas turbine applications. Also, a new ammonia combustion concept from Siemens Energy is currently ongoing for testing in CARES using the Swirl burner.

OTHER ACTIVITIES AND ACHIEVEMENTS

The conference participation by HYCOMBS is listed below:

- Dr Li Chin LAW (Research Fellow, CARES) had an oral presentation "Economics of hydrogen-fuelled vessel: A stochastic techno-economic framework under price & regulatory uncertainty" at the Singapore Maritime Research Conference from 22 - 23 April 2026 in Singapore
- Dr Yong Ren TAN (Research Fellow, CARES) presented a poster "The effects of non-premixed hydrogen on soot formation in an ethylene-fuelled laboratory-scale rich-quench-lean combustor" at the Singapore Maritime Research Conference from 22 - 23 April 2026 in Singapore
- Dr Yuxi GUO (Research Fellow, NTU) had an oral presentation "Numerical study on combustion and emissions in a premixed ammonia–diesel dual-fuel engine with varied diesel injection strategies" at the International Conference on Materials and Energy from 10 - 12 June 2026 in Corte, France
- Dr Tan had an oral presentation "The effects of non-premixed hydrogen on soot formation in an ethylene-fuelled laboratory-scale rich-quench-lean combustor" at the ASME Turbo Expo from 15 - 19 June 2026 in Milan, Italy
- Dr Hao YAN (Research Fellow, NUS) had an oral presentation "Numerical investigation of the interaction between vortex pair and detonation" at the Tenth International Symposium on Physics of Fluids from 19 - 23 June 2026 in Fuzhou, China
- The World Hydrogen Energy Conference (WHEC 2026) from 22- 26 June 2026 in Singapore saw several oral presentations from HYCOMBS:
  - Dr Zifeng WENG (Research Fellow, NUS), "Chemical inhibition of hydrogen detonation using trifluoroiodomethane (CF_3I) addition"
  - Dr Guo, "Effects of strut geometry on combustion and emission characteristics in a hydrogen fueled trapped vortex combustor"
  - Dr Yan, "Numerical investigation of detonation interaction with a vortex"
  - Dr Xin LI (Research Fellow, NUS), "Evolution of double-layer hydrogen gas cylinder induced by a convergent shock"
  - Dr Law, "A two-layer stochastic techno-economic framework for hydrogen-based maritime decarbonisation under market and policy uncertainty"
  - Dr Francesco D'ALESSIO (Research Fellow, CARES), "Evaluation of heat release rate markers for partially cracked ammonia combustion with air"
  - Dr Hao SHI (Research Fellow, CARES), "Laminar burning velocity and Markstein length of high-pressure NH_3/H_2/air premixed flames: A comparitive numerical study
- Dr Guo had an oral presentation "Effects of diesel injection strategies on combustion and emission characteristics of a tri-fuel engine" at the 7th International Symposium on Thermal-Fluid Dynamics from 10 - 13 July 2026 in Xi'an China. Dr Guo also received the Best Paper Award for the work on the study of the effects of injection strategy on combustion and emissions in a diesel-ignited ammonia-methane engine
- Dr Shi had an oral presentation "Laminar burning velocity and Markstein Length of high-pressure NH_3/H_2/air premixed flames: A comparative numerical study" at the Decarb Researcher's Seminar Series on 16 July 2026 in the CREATE Tower, Singapore
- The 41st International Symposium on Combustion from 26 – 31 July 2026 in Kyoto, Japan saw several presentations from HYCOMBS:
  - Dr Weng had an oral presentation "Detailed modelling of hydrogen detonation initiation inhibited by trifluoroiodomethane"
  - Dr Aksel ÅNESTAD (Research Fellow, CARES), had an oral presentation "The effect of interference between axially staged flames on thermoacoustic stability"
  - Prof Christine MOUNAÏM-ROUSSELLE (PI, CNRS) and Prof Huangwei ZHANG (PI, NUS) had a joint oral presentation "Direct uncertainty quantification of high-dimensional combustion kinetic models through deep reinforcement learning"
  - Dr Nader SHOHDY (Research Fellow, CNRS), presented a poster "Temperature and H2O mole fraction fluctuations in oscillating NH_3/CH_4 flames measured by laser absorption spectroscopy"
  - Dr Jintao CHEN (Research Fellow, CARES), had an oral presentation "An experimental and kinetic modelling study of the ignition of tert-amyl methyl ether'
  - Dr Shi had an oral presentation "In-cylinder knock diagnostics of a spark-ignition engine using deep learning-based optical flow and flame luminosity"
  - Dr Tong SU (Research Fellow, CARES), presented a poster "Structure and extinction of CH_4-air swirl flames with premixed and non-premixed hydrogen injection"
  - Dr Victor LAFAURIE (Research Fellow, CARES), presented a poster "Numerical and experimental study of ignition and fame dynamics of NH_3/H_2 with various chemical kinetics using a micro flow reactor with a controlled temperature profile"



A group photo of HYCOMBS members at the 41st International Symposium on Combustion in Kyoto, Japan.

In April 2026, HYCOMBS researchers participated in the Expo component of Singapore Maritime Week from 21 - 23 April with a booth that welcomed industry visitors to learn more about the research and discuss collaboration opportunities. This year's event welcomed more than 34k attendees from over 80 participating countries. In the same month, the team also conducted a 2-day training workshop, called HYCOMBS School, that introduced the combustion concepts that HYCOMBS was advancing to the academic community and industry engineers from Hanwha Power Systems and Siemens Energy.



From left to right: Dr B Harirksihnan, Iffah Azlin (Comms team), Mei Qi Lim, Dr Li Chin Law, Dr Marc Le Boursicaud, Olivia Lee (Comms team), Prof Epaminondas Mastorakos, and Dr Yichen Zong.



Guests visiting the HYCOMBS booth at Singapore Maritime Week 2026.



Attendees at HYCOMBS School participated in 2 days of presentations and had the option to join a lab visit.



SM3

SUSTAINABLE MANUFACTURE OF MOLECULES AND MATERIALS IN SINGAPORE

SM3 will aim to shift the chemical manufacturing industry to a more circular, sustainable, and resilient model. This project will address systemic challenges, including the integration of regionally available resources and the development of scalable, flexible technologies for local manufacturing.

Project Leads











THEME 1: NOVEL SYNTHETIC STRATEGIES

WP1. Novel Synthesis Methods

Prof Ning YAN (NUS)
Dr Jiong CHEN (NUS)

We developed two complementary routes for converting biomass-derived feedstocks into value-added building blocks while preserving or redirecting their inherent functionality. First, a ReOx/activated-carbon (ReOx/AC) catalytic system was developed for the selective 2,3-deoxydehydration of carbohydrate-derived sugar acids. The transformation preserves the remaining stereogenic centres and affords chiral vicinal diols bearing two defined stereocentres (Figure 2.1). These products are versatile intermediates for downstream asymmetric synthesis, as demonstrated in a biomass-based route to (+)-muricatacin.

The chiral diols can also serve as substrates for transformations developed by Prof Ming Joo KOH's (PI, NUS) team, while their sugar-deoxygenation chemistry could in turn supply deoxygenated sugar-acid precursors, expanding the library of accessible chiral building blocks. The (+)-muricatacin route will also be used as a case study in the cheminformatics framework developed in WP2, linking upstream biomass feedstocks with downstream synthesis.

Second, we elucidated a reaction network for converting chitin-derived aminogluconic acid into amino acids through an artificial transamination process. In a metal–pyridoxal (PL) system, aminogluconic acid first undergoes retro-aldol cleavage to glycine and erythrose. Glycine then reacts with PL to form the corresponding pyridoxamine intermediate, enabling subsequent transamination and opening a route toward a broader amino-acid library.

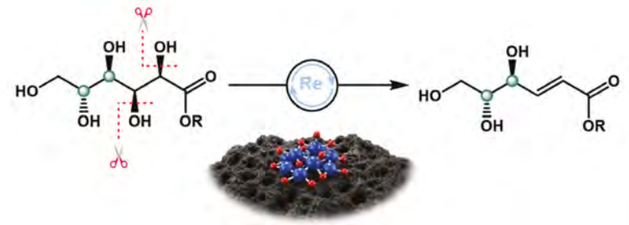


Figure 2.1: Transfer of biomass-encoded chirality

Prof Ming Joo KOH (NUS)
Dr Jun WU (NUS)

This period, we substantially advanced our photocatalytic "lock-and-cut" strategy for site-selective deoxygenation of carbohydrates, focusing on reaction generality, the origin of selectivity, synthetic utility and scalability (Figure 2.2). The substrate scope now covers 13 monosaccharides, two disaccharides, one trisaccharide, two nucleosides, five sugar derivatives and glycosides bearing eight different aglycones. Deoxygenation can be directed to the C2, C3, C4 or C6 position, and multiple deoxygenations are possible, including four examples of double deoxygenation and one quadruple deoxygenation.

Mechanistic studies combining light on/off experiments, Hammett analysis, quantum-yield measurements and DFT calculations gave further insight into the photochemical pathways and helped rationalise the observed site selectivity. The method's utility was demonstrated in a streamlined synthesis of the repeating tetrasaccharide unit of the O-chain from a phytopathogenic bacterium: a late-stage quadruple deoxygenation delivered the target in 14 steps, compared with 24 steps in the previous synthesis. The manuscript describing this work is under peer review.

In parallel, we are working with Prof Saif A. KHAN's (PI, NUS) team in (WP3) to translate the batch photochemistry into scalable flow processing. Our photocatalytic coupling of unprotected sugars with N-heteroarenes, which gives medicinally relevant C-heteroaryl glycosides in a single operation, has now been published in *Nature Synthesis.*

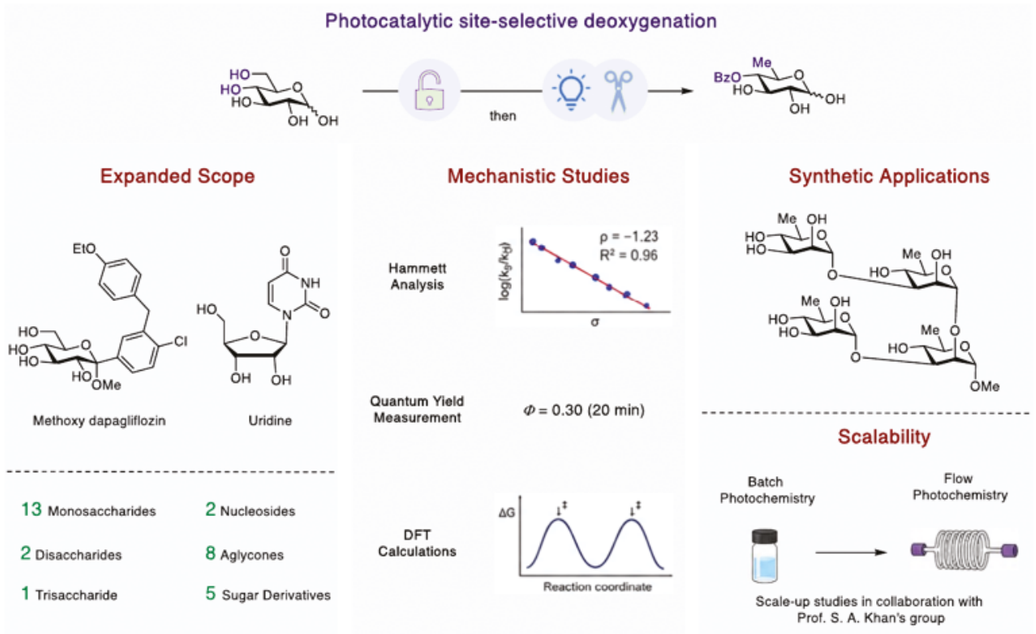


Figure 2.2: Progress of the photocatalytic "lock-and-cut" strategy for site-selective carbohydrate deoxygenation and ongoing flow-chemistry scale-up with Prof Saif Khan's group.

Prof Shunsuke CHIBA (NTU)
Dr Taku WAKABAYASHI (NTU)

Nitrogen-containing heteroarenes, particularly diazines (six-membered dinitrogen aromatics) and diazoles (five-membered dinitrogen aromatics), are widely found in modern medicines and agrochemicals. Strategically modifying these core frameworks allows bioactive chemical space to be diversified without the constraints and resource intensity of de novo assembly.

During this period, we developed photocatalytic methods that directly transform diazines into diazoles: pyrimidines (1,3-diazines) into imidazoles (1,3-diazoles), and pyridazines (1,2-diazines) into pyrazoles (1,2-diazoles) (Figure 2.3). The key to this strategy is photocatalytic single-electron transfer to access dearomatised diazacyclohexadienyl anions, which undergo ring contraction via disrotatory 6π-1,5-electrocyclisation. This work has been accepted in the *Journal of the American Chemical Society* and could open previously untapped chemical space for drug and agrochemical discovery.

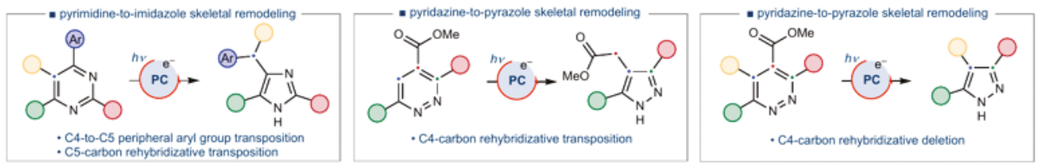


Figure 2.3: Pyrimidine-to-imidazole and pyridazine-to-pyrazole skeletal remodelling via photoredox catalysis.

Prof Matthew GAUNT (CAM)
Dr Rakesh MAITI (CARES)

One-carbon ("1-C") homologation can profoundly influence the biological activity of a molecule by altering its size, conformation and spatial arrangement. The immunosuppressant tacrolimus (FK-506), for example, owes much of its activity to the length of its hydrocarbon side chain relative to its homologues FK-523 and FK-520. We previously developed a "1-C" reagent that inserts a methylene (–CH_2–) unit into acyclic alkenes through a one-pot cross-metathesis and acid-mediated fragmentation sequence.

We are now extending this concept to cyclic alkenes, where inserting one carbon changes the ring size. Ring expansion is a well-established strategy in medicinal chemistry; "1-C" ring expansion of GPR119 agonists, for instance, significantly changes their potency. We are exploring a one-pot cyclopropanation/ring-opening strategy, although the controlled opening of the cyclopropane to regenerate the alkene with one extra carbon remains an elusive transformation.

To identify a viable pathway, we collaborated with the SM_3 AI team, Prof Tej CHOKSI (PI, NTU), Prof Philippe SCHWALLER (PI, EPFL), Dr Karam HASHEM (Research Fellow, NTU) and Dr Ka Lok CHAN (Research Fellow, CARES). Thermodynamic and kinetic calculations on carbocation, radical and carbanion pathways showed the carbanionic route to be the most favourable (Figure 2.4a). This guided the design of a bifunctional "1-C" reagent combining a diazo group for the initial cyclopropanation with a TBS-protected sulfone that stabilises the diazo group and helps generate the carbanionic intermediate (Figure 2.4b). The reagent has been synthesised from inexpensive, commercially available rongalite through TBS protection followed by a three-step sequence installing the diazo group (Figure 2.4c). We are now optimising the cyclopropanation step before moving on to the ring-opening/rearrangement.

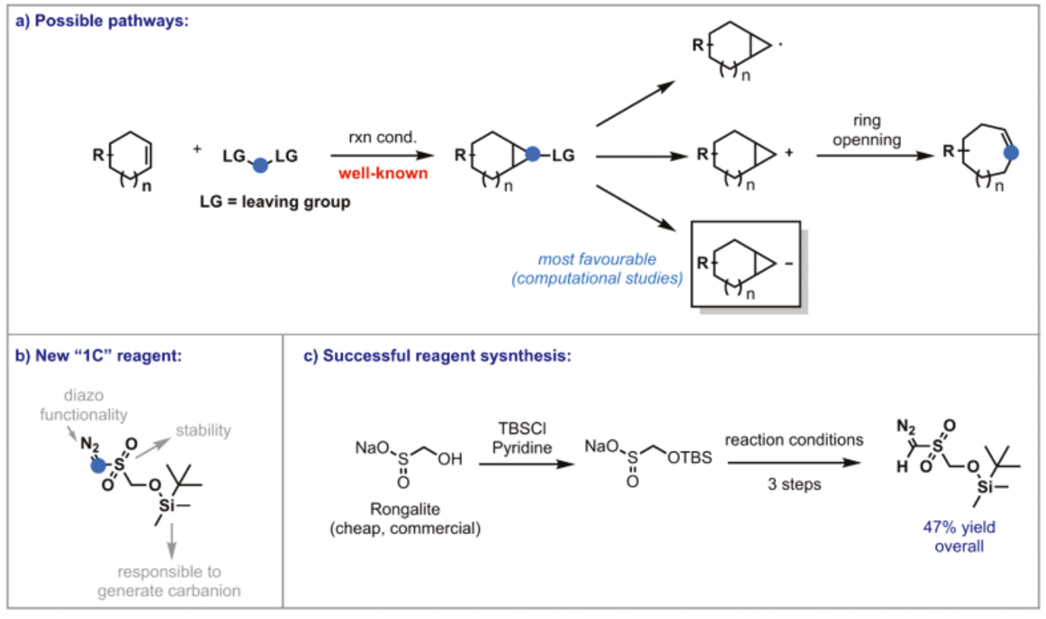


Figure 2.4: (a) Determination of the favourable pathway, (b) design of the new "1-C" reagent, (c) synthetic pathway.

WP2. Reaction Networks and Project Targets

Prof Alexei LAPKIN (CAM)
Dr Raudah LAZIM (CARES)

Valorising biomass requires knowing which target compounds can actually be reached from a given feedstock through real chemistry. We developed a knowledge-based computational workflow that identifies such targets by tracing synthetic routes through a directed bipartite reaction graph, built from a large corpus of organic reactions curated from the Reaxys database. Molecules and reactions are represented as nodes connected as reactant → reaction → product, so a product is only reachable if all the necessary reactants are available. The traced pathways therefore correspond to chemically consistent reaction sequences rather than simple molecule-to-molecule connections.

Starting from biomass-derived feedstocks, we traverse the network downstream and assess candidate routes with chemically informed progression criteria rather than shortest paths alone. Route progression is currently evaluated with the unnormalised Spatial Score (SPS), an additive complexity descriptor calculated in RDKit from each heavy atom's hybridisation, stereochemistry, ring membership, and neighbour count. Stepwise changes in SPS (ΔSPS) favour routes that steadily build up the tracked scaffold, with a defined tolerance for small decreases to accommodate essential steps such as protection, deprotection and functional-group interconversion. Next, we will add the normalised SPS (SPS divided by the number of heavy atoms) and a measure of synthetic difficulty to rank routes before costlier computational or experimental validation.

Reachable products are screened along two independent dimensions. Pharmaceutical relevance is assessed against the WHO Model List of Essential Medicines (EML) using exact structural identity, shared core scaffolds and fingerprint-based similarity. Polymer relevance is assessed by identifying reactive functional groups associated with major polymerisation mechanisms. Both analyses are automated, allowing systematic screening of the reachable chemical space without manual structural review.

The workflow is illustrated in Figure 2.5 using succinic semialdehyde, investigated with Prof Ruth WEBSTER's (PI, CAM) team. Within three reaction steps, no exact matches to the WHO EML were found, but several targets shared core scaffolds with listed drugs across multiple therapeutic classes. Functional-group scanning also identified products compatible with polyesters, polyamides and polyethers. The search recovered γ-aminobutyric acid (GABA), used as a positive control, and tetrahydrofuran (THF), showing that the workflow finds both biologically relevant molecules and industrially important intermediates.

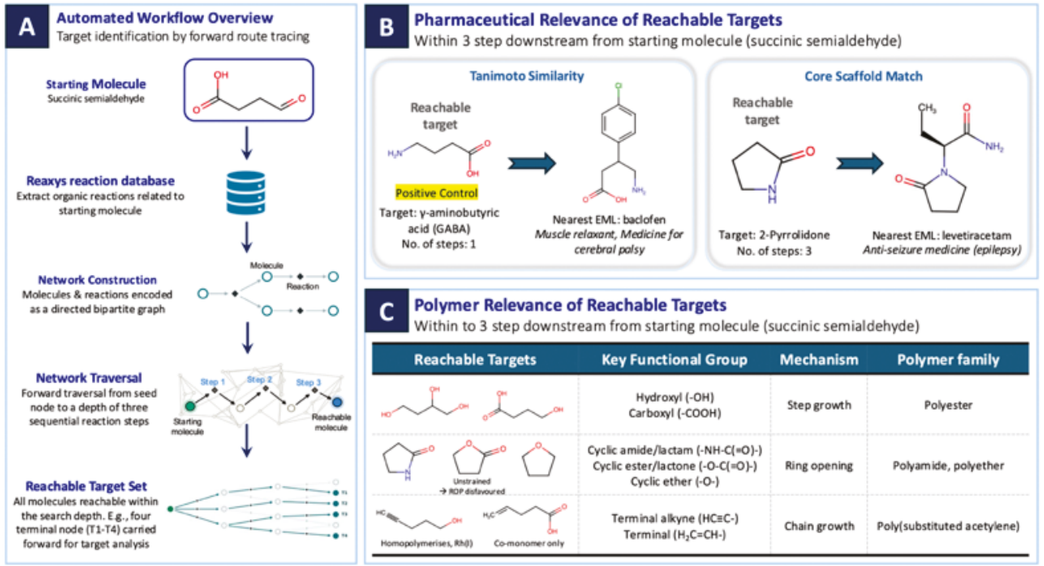


Figure 2.5: (A) Overview of reaction network traversal used for target identification. (B) Representative targets reachable from succinic semialdehyde within three forward steps, matched against the WHO EML by Bemis–Murcko scaffold matching or nearest-neighbour Tanimoto similarity. GABA serves as a positive control. (C) Reachable targets with functionalities relevant to major polymerisation mechanisms, with the accessible polymer families and their limitations.

Prof Ruth WEBSTER (CAM)
Dr Miguel CHACON-TERAN (CARES)

Building on the feedstock strategy established in the previous reporting period, which identified acid whey as a source of glutamic acid, we have moved from resource identification to transformational synthetic chemistry. Glutamic acid is now used as a common platform for the production of high-value specialty chemicals and functional biopolymers.

We have demonstrated several new single-step transformations at multigram scale, giving L-pyroglutamic acid, 3-cyanopropanoic acid and succinic semialdehyde (Figure 2.6). Sustainability and techno-economic considerations were built in from the outset, with a focus on process intensification, reduced solvent demand, efficient resource use and closed-loop reagent regeneration where applicable. Together, these routes show how a widely available commodity amino acid can be upgraded into specialty products for pharmaceutical, personal-care, biochemical and advanced-material applications.

In parallel, we have developed a chemical route to poly-γ-L-glutamic acid, a biodegradable functional polymer with potential applications in pharmaceuticals, drug delivery, cosmetics and advanced materials. The route has been demonstrated at the 100 g scale and is progressing toward kilogram scale. Current work focuses on scale-up, process optimisation, product performance, intellectual-property generation and commercial validation. These results lay the foundations of an amino acid-based specialty chemicals and biopolymers platform that could support industrial partnerships, technology transfer and future venture creation.

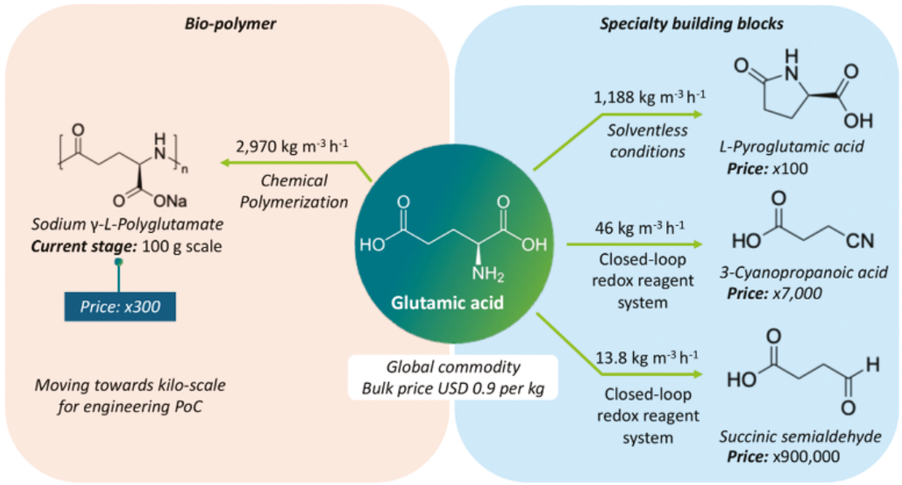


Figure 2.6: Value upgrading of glutamic acid into high-value specialty chemicals and poly-γ-L-glutamic acid. Current developments span multigram-scale specialty-chemical synthesis and 100 g polymer production, combining high process productivity with solventless or closed-loop processing. Price multipliers indicate representative market-value differences relative to commodity MSG. Space-time yield expressed in kg m^{-3} h^{-1}.

THEME 2: SCALABLE AND SUSTAINABLE TECHNOLOGIES

WP3. Novel Scalable Synthesis Technologies

Prof Saif KHAN (NUS)
Fangyuan ZHANG (NUS)
Yi Wei LEE (NUS)

WP3 is developing a dedicated scale-up workflow for the novel synthesis technologies emerging from Theme 1. In the previous reporting period, we set out a three-stage workflow: (i) kg-scale reactor design and fabrication, (ii) operational regime mapping using our algorithmic "Regime Cartography" framework (RCF), and (iii) intra-regime optimisation. The workflow is being tested using a model electrochemical aryl amination reaction (accepted, *Nature Communications* 2026).

Over the past six months, we completed Stage 1 and began Stage 2. A major deliverable was the design, fabrication and commissioning of a kilogram-scale tubular electrochemical flow reactor (TEFR). The electrode geometry was optimised by computational fluid dynamics (CFD) to increase surface area and improve fluid mixing, and, given the complexity of the design, the electrodes were fabricated by selective laser melting. The fully operational kg-scale TEFR system is shown in Figure 2.7.

With the reactor complete, we have begun implementing the RCF, a data-driven framework that partitions the reactor operating space into regimes, each representing quantifiably different reactor behaviour. Experimentally, we have identified the operating-parameter boundaries for regime mapping and are refining protocols to ensure reproducible reaction outcomes. Algorithmically, we developed a new workflow to quantify the similarity between NMR spectra of TEFR reaction products that accounts for the size of chemical-shift differences, a capability required to identify operating regimes within the RCF.

Beyond the main scale-up programme, the TEFR platform is being evaluated under the Max-CREATE-SCCB initiative for continuous-flow production of biomass-derived platform molecules, with batch-to-flow translation under way (Dr Huang Ningyu and Dr Jakob Wolf are involved, as researchers from the Max Planck Institute). Scale-up of the photochemical transformations developed by Dr Jun WU (Research Fellow, NUS) in kilo-scale photoreactors is also progressing, with reaction temperature being optimised in automated Vapourtec flow reactors before deployment at kilogram scale.

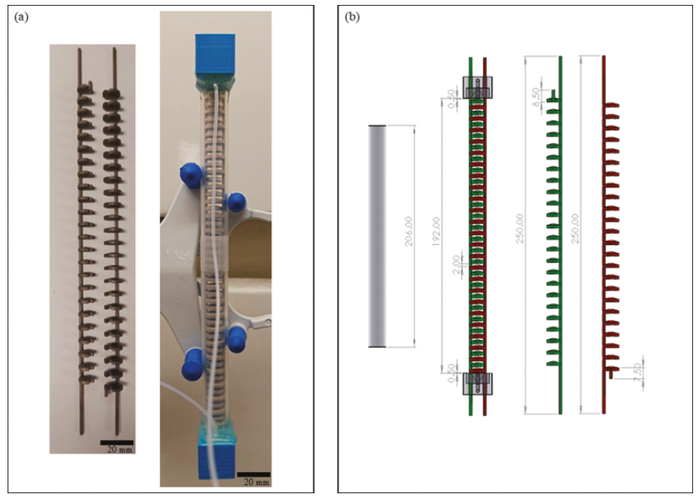


Figure 2.7: (a) Electrodes created via selective laser sintering and assembled into the operational TEFR. (b) Schematic drawing of the assembled TEFR.

WP4. Technology Mapping and Value Chain Analysis

Prof Alexei LAPKIN (CAM)
Dr Pavlos GKINIS (CARES)

We have developed a technology map that categorises and parametrises manufacturing technologies for multi-product pharmaceutical production, identifying the minimum set that covers all or most process steps for selected products. It answers which technologies, at what scale and containment level, can cover a chosen portfolio of active pharmaceutical ingredients (APIs), and how different products can share a plant. Decisions normally made by expert estimation become explicit, auditable queries over structured data, which will feed the library of process models and the evaluation of sustainability indicators.

The first full version was built and deployed this period in three layers, using a limited dataset. An ontology encodes 100 APIs and their published synthesis routes step by step, with 22 unit operations parametrised by process capability and product-level classes for scale, containment and potency (Figure 2.8). A deterministic reasoning engine (owlready2) computes minimum equipment sets for chosen APIs or portfolio fractions, modifications of existing plant, overlaps through shared chemicals and multi-product compatibility flags. These sit within a web application with structured tools and a free-text query box, making the map usable by non-specialists. An optional language model, cloud-based or fully local, only parses questions and narrates answers; every output is computed deterministically.

An initial taxonomy study classified all transformations under a published industrial reaction hierarchy (Carey et al., *Org. Biomol. Chem.* 2006). It showed that reaction class and subclass, combined with condition flags, could be the basis for automated equipment assignment of newly added chemistry.

Because solvents dominate process mass and waste in drug-substance manufacture, we also delivered the map's first sustainability indicator: a merged solvent guide that normalises the GSK guide (Henderson et al., *Green Chem.* 2011; Alder et al., *Green Chem.* 2016) and CHEM21 (Prat et al., *Green Chem.* 2016) onto one safety, health and environment frame. It covers 160 solvents with a single verdict each and reimplements the published methodology, so solvents outside both guides can also be scored.

Forthcoming work includes expanding toward a database of more than 3,000 APIs, with processes assigned from published manufacturing recipes and automated through taxonomy and condition similarity to annotated precedents. Solvents will be attached to each step so that routes and portfolios can be scored for sustainability and greener substitutions suggested, in collaboration with WP2 and WP5. Techno-economic analysis with CAPEX/OPEX estimates per product, in collaboration with WP6, will place cost alongside unit count in plant-design decisions.

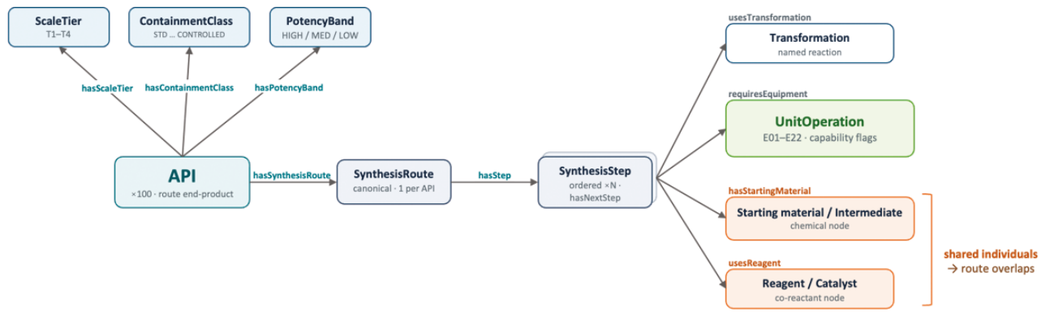


Figure 2.8: Knowledge graph structure: 100 drug substances (first integration), their synthesis routes and a catalogue of 22 process unit operations encoded as a single queryable ontology (~2,770 individuals).

THEME 3: SUSTAINABILITY, SYSTEMS AND AI

WP5. AI for Chemistry

Prof Tej CHOKSI (NTU)
Dr Karam HASHEM (NTU)

Reaction-network thermochemistry turns a proposed synthetic route into a quantitative object. Knowing the free-energy change of every step shows which transformations are feasible, which are thermodynamically marginal and therefore sensitive to conditions, and which side reactions are likely to generate impurities. The last point is decisive in pharmaceutical manufacture, where impurity control governs regulatory acceptability as much as yield governs cost. Building this layer computationally allows routes to be screened at the scale at which the WP2 workflow proposes them.

Over the last six months, we developed and consolidated a computational thermochemistry framework, using the reaction networks for gefapixant synthesis as a case study. This included establishing the workflow in the Chemical Data Intelligence (CDI) Lab environment, with ORCA-based DFT calculations and automated or semi-automated procedures for structure preparation, geometry optimisation, frequency calculations, job submission, restarts and status monitoring. We also developed a literature-to-input workflow using DECIMER and MolScribe to extract molecular structures from PDFs and convert them into ORCA input files, reducing manual transcription and complementing future integration with CDI's DISTILL capabilities.

We applied the workflow across three reaction networks, most recently completing and validating Network 3 (Figure 2.9a). Species identities, reaction stoichiometry and experimentally relevant conditions were consolidated so that reaction thermodynamics could be evaluated under conditions representative of the reported chemistry. The resulting free-energy landscape helps identify favourable and unfavourable transformations and prioritise potentially important synthetic and impurity-forming pathways. The work links reaction-network mapping in WP2, mechanistic input from the synthetic chemists, transition-state and kinetic analysis with Prof Schwaller's team, and process metrics in WP4 and WP6 (Figure 2.9b).

Separately, our recent publication in *ACS Sustainable Chemistry & Engineering* combines experimental mechanochemistry with computational modelling to develop a greener route for recycling polyethylene terephthalate (PET) waste. K_2CO_3-catalysed mechanochemical methanolysis depolymerises PET rapidly at room temperature, with high conversion and selectivity toward dimethyl terephthalate (DMT), and DFT calculations clarify the catalytic role of methoxide formation.

Next, we will finalise the three-network thermodynamic dataset and prioritise key reactions and impurity pathways. In parallel, we are launching an integrated computational platform with Dr Raudah Lazim, Dr Chunchu Balaji and Dr Ka Lok Chan to connect reaction-network exploration, thermodynamics, mechanistic modelling, transition-state searches and kinetics.

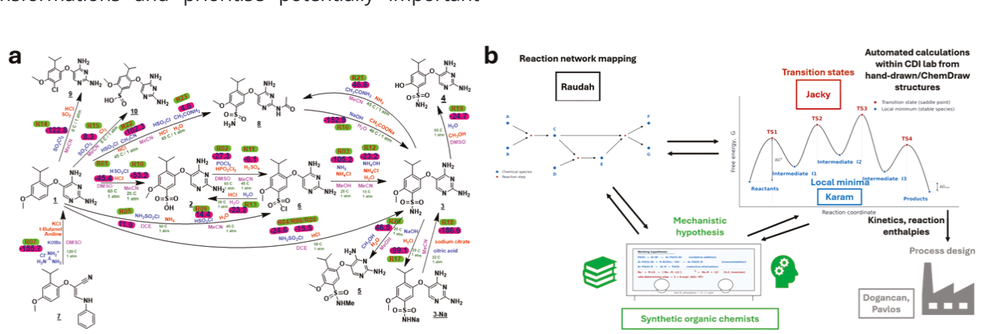


Figure 2.9: (a) Thermodynamic mapping of gefapixant reaction Network 3, showing calculated reaction free energies with the reagents, solvents, temperatures and pressures used for each step. (b) Planned collaborative framework within SM_3 linking reaction-network mapping, mechanistic hypothesis generation, thermodynamic calculations, transition-state and kinetic analysis, and process-level interpretation.

Prof Philippe SCHWALLER (EPFL)
Dr Ka Lok CHAN (CARES)

We developed an agent-based multi-agent framework for automated transition-state (TS) search in homogeneous reactions. Multi-step DFT workflows are orchestrated through a Large Language Model (LLM)-powered ReAct (Reasoning and Acting) loop: user prompts are parsed and executed as structured steps, and the agent iteratively reasons about progress, decides on next actions and carries them out.

Several new toolsets support the framework. A TS Finder generates initial TS guesses through constrained optimisation. A Constrained Optimiser enables LLM-guided and Gaussian Process Regression-guided refinement, proposing improved trial geometries based on previous attempts. A Task Resubmission tool parses error-terminated jobs, reconstructs input geometries and resubmits them, closing the loop between failure detection and recovery. A Quality Evaluation tool judges the results of constrained and TS optimisations from both chemical and optimisation perspectives to guide candidate selection.

The framework applies to homogeneous reactions with multiple bond-breaking or bond-forming events that can be expressed as reaction SMARTS (Figure 2.10). It proceeds from an initial TS guess, through iterative refinement and error handling, to full TS optimisation of promising candidates and validation by Intrinsic Reaction Coordinate calculations, which confirm that the TS connects the intended reactant and product. Once initiated, the workflow runs autonomously, which is crucial for high-throughput exploration of reaction pathways.

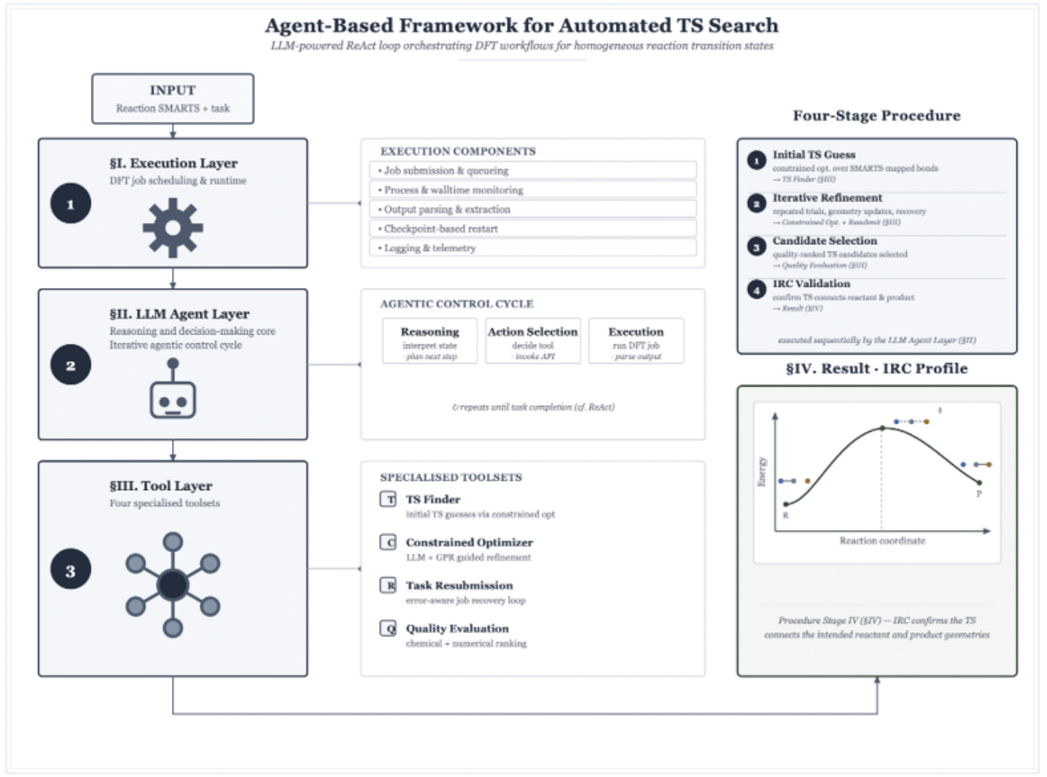


Figure 2.10: Schematic of the steps in the agent-based framework for automated transition-state search.

Prof Tej CHOKSI (NTU)
Dr Neeru CHAUDHARY (NTU)
Dr Chunchu BALAJI (NTU)

We developed and applied an integrated workflow combining a machine-learning interatomic potential with DFT for transition-state identification and mechanistic exploration of catalytic reactions involving large multifunctional molecules. The hybrid MACE–DFT framework accelerates TS searches while retaining DFT-level accuracy. We applied it to the hydrogenation of p-chloronitrobenzene and nitrobenzene on Pd(111), industrially important routes to pharmaceutical intermediates. Benchmarked against conventional DFT, the workflow reliably predicted TS geometries, vibrational frequencies and activation barriers, with a mean absolute difference below 0.1 eV, at one third of the computational cost.

We are now extending the approach to the conversion of methoxyphenol to methoxyaniline, an SM_3-relevant reaction (WP1) with multiple competing hydrogenation, deoxygenation, amination and dehydrogenation pathways. With Dr Jiong CHENG (Research Fellow, NUS) and Prof Ning YAN (PI, NUS), we are combining DFT insights with experimental observations to understand the selectivity between C–O bond scission and C–H bond formation during methoxyphenol hydrogenation (Figure 2.11). A collaborative manuscript on the accelerated TS-search workflow is in preparation.

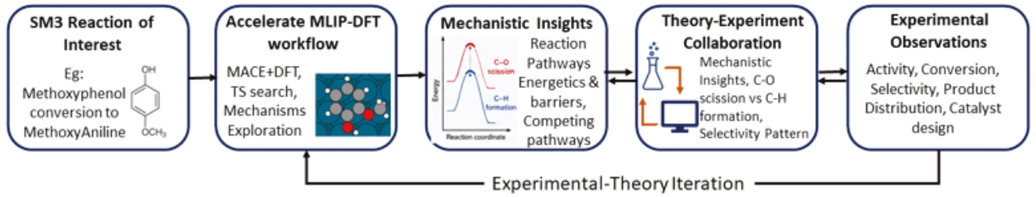


Figure 2.11: Integration of the machine learning-accelerated DFT workflow for mechanistic exploration with experiments on catalytic reactions within the SM_3 consortium.

WP6. Metrics and Systems

Prof Ewa MAREK (CAM)

Dr Lek Hong LIM (CARES)

Choosing the most economical pathway from feedstock to product means comparing many candidate synthesis routes with each comparison needing a cost estimate. These estimates are slow to produce, and published ones rarely use the same assumptions, so routes are hard to compare. Building on our modular cost-estimation framework, we can now construct the process model, size the equipment and estimate the economics automatically, so that every route is assessed the same way.

The framework can check published studies quickly: we rebuilt a published process model and its economics from the paper alone, and the product cost agreed within 4% (Figure 2.12a). It compares routes on the same assumptions, including production capacities, utility prices, financial parameters, battery limits, and costing methods, so that cost differences reflect the chemistry and the process rather than how each estimate was made. It also shows how uncertain a cost estimate really is. We combine six published costing sources for each equipment type, and they disagree far more than is usually acknowledged (Figure 2.12b); in the validation study, the published cost sat at the low, optimistic end of the range the methods allow.

The framework complements the WP4 technology map, which matches each step of a synthesis route to the process technologies that can perform it. The framework prices whatever the map proposes, including novel equipment without historical cost data, which is costed from its design weight and how difficult it is to fabricate. In return, it tells the map which technologies are feasible at the required scale. Together, they could compare and rank synthesis routes without manual modelling in between.

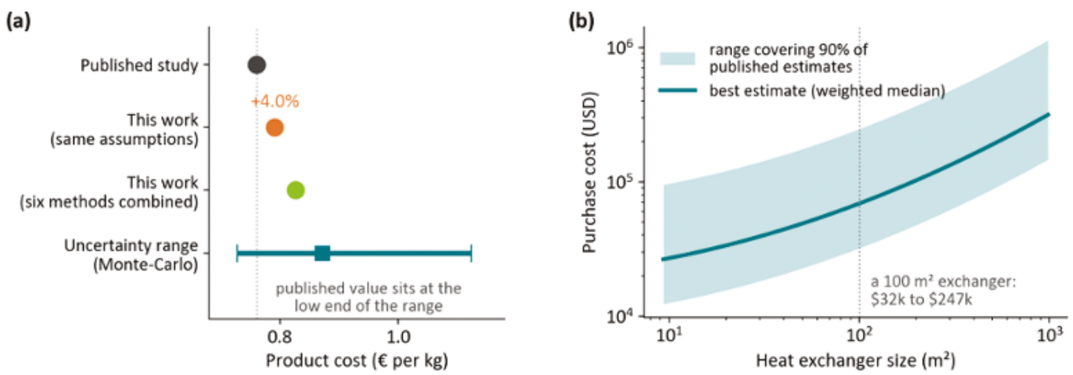


Figure 2.12: (a) A published study rebuilt by the framework: the cost agrees within 4%, and the range from six costing methods shows that the published value is optimistic. (b) Cost of a floating-head shell-and-tube heat exchanger according to four published sources. The line is the weighted median (by source relevance, age and extrapolation distance) and the shaded band covers 90% of the estimates.

Prof Markus KRAFT (CAM)

Dr Kumaran ELUMALAI (NTU)

We are creating digital twins of the high-throughput experimentation (HTE) systems being built at NTU under SM_3, to enable predictive, interoperable and sustainability-aware workflows. A modular ontology stack captures laboratory infrastructure, equipment, scheduling, documentation, maintenance and spatial allocation. We reuse existing ontologies such as OntoLab, OntoDevice, OntoReaction and OntoAssetManagement where possible, and are developing two new ontologies, OntoHTE and OntoOpentrons, for HTE-specific requirements. By integrating these ontologies, we built a draft digital twin of a photochemical reaction setup (Figure 2.13).

In parallel, we are developing reusable catalysts for API synthesis. The synthesis of dapagliflozin from hub molecules relies on homogeneous catalysts, including nickel. Anchoring the active metal onto metal–organic frameworks (MOFs) or metal–organic polyhedra (MOPs) turns it into a heterogeneous catalyst that can be recovered and reused. Inspired by the work of Prof Koh we synthesised Ti- and Zr-based MOFs containing $NiCl_2$ through MOF synthesis followed by post-functionalisation, and confirmed their structure by infrared spectroscopy and powder X-ray diffraction. We also collaborate with Prof Choksi on the AI-predicted synthesis of novel metal–organic polyhedra within The World Avatar.

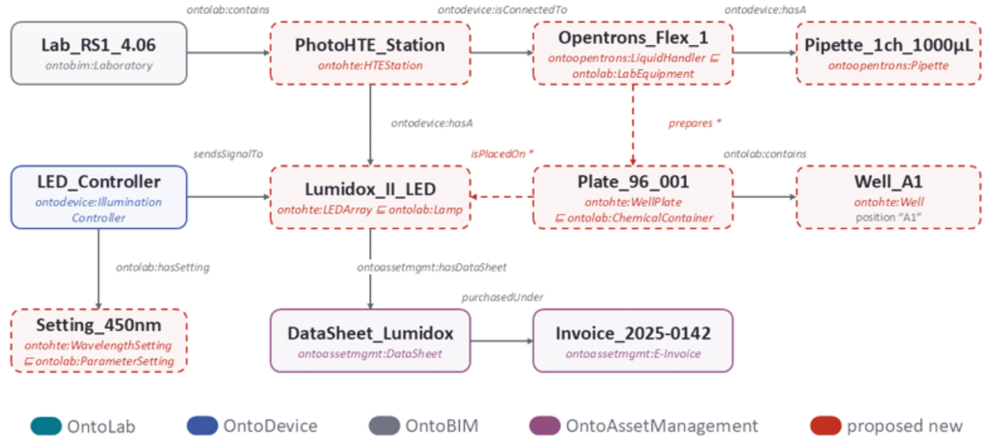


Figure 2.13: Draft digital twin of a photochemical reaction setup for HTE.

OTHER ACTIVITIES AND ACHIEVEMENTS

Prof Alexei LAPKIN (PI, CAM) gave an invited talk, "The role of AI in transition to sustainable chemistry", at the Gordon Green Chemistry conference from 26 - 31 July 2026 in Spain. He also gave a plenary talk, "(SM_3) Sustainable Molecules and Materials Manufacture – design of complete chemistry value chain for 'net-zero chemistry'", at the Transforming Chemistry Summit from 15 - 16 September 2026 in Leipzig, Germany.

Dr Chunchu BALAJI (Research Fellow, NTU) presented the poster "Accelerating Transition-State Searches and Potential Energy Surface Exploration via Machine Learning Potentials and First-Principles Calculations" at the Singapore Catalysis Forum 2026, held at NTU on 28 July 2026.

The Taiwanese chemicals manufacturer Everlight Chemical has joined the CARES-based centre in Digital Molecular Technologies. Its senior managers will join the SM3 workshop in October 2026 to discuss shared challenges in de-fossilising chemicals manufacturing and to identify collaborative sub-projects.

SM_3 is now co-led by Prof Lapkin and Prof Saif A. KHAN (PI, NUS), with a programme manager joining on 1 July 2026 to coordinate activities across the project.



HD4

HEALTH-DRIVEN DESIGN FOR CITIES

HD4 will investigate how individuals live and move in Singapore, how the urban environment shapes their exposure to health risks and how this influences their behaviour and health.

People living in cities face growing challenges to their health and wellbeing, including heat, noise, air pollution, and limited opportunities for a healthy diet and physical activity. Understanding how the design and organisation of cities influence health is an important priority in Singapore.

HD_4 brings together researchers from Nanyang Technological University, the National University of Singapore, and the University of Cambridge. The programme adds environmental exposure information to SG100K, Singapore's national longitudinal cohort. This allows behavioural and health data, including information linked from electronic health records and national disease registries, to be analysed in relation to the environments in which participants live and move.

Singapore provides a unique setting for this research. With ambitious public health goals, rich data resources, and a strong commitment to evidence-informed urban planning, Singapore offers an exceptional opportunity to study how urban environments influence health. Working in partnership with government agencies, HD_4 aims to generate insights that can help guide future strategies for designing healthier cities.

Research Plan

HD_4 works in partnership with SG100K to understand how Singapore's urban environment shapes health-related behaviours and long-term health. By combining detailed environmental measures with longitudinal behavioural and clinical data, the programme can examine how the environments in which participants live and move relate to their behaviour and health.

HD_4 is being implemented in phases. Phase 1, funded from November 2024 to April 2027, is establishing the environmental data, linkage methods, analyses, participant studies and agency partnerships needed for this research. Phase 2 will build on these foundations and concentrate on scientific and agency problems where new evidence can inform policy and planning in Singapore.

HD_4 has shown that national-scale environmental data from existing sources can be collated, converted into traceable participant-level exposure measures and linked to SG100K. Measures of green space, humid heat, and walking and cycling accessibility are now linked, with humid heat and walking and cycling accessibility added during Q2 and Q3 of 2026. Food-retail measures and environmental archetypes are being prepared for linkage. The source data were selected to overlap in time with SG100K, allowing each analysis to align environmental exposures with the relevant periods of behavioural and health data.

Work is in progress to analyse how these exposures relate to physical activity, sleep, diet, and cardiometabolic health, using SG100K data and linked health records. Focused participant studies are developing methods for measuring location and movement, indoor environments, fitness, physical function, and diet in daily life. Engagement with Singapore agencies is helping to identify the questions and evidence needs that will guide the remaining Phase 1 work and the development of Phase 2.

"This project will develop the science of connecting the environment with health at multiple scales, from how individual Singaporeans experience the city, to how planners and policymakers shape our urban futures."

Professor Ronita Bardhan
Deputy Programme Lead, CAMBRIDGE

Dr Rudi Stouffs
Deputy Programme Lead, NUS

Project Leads


Professor Nick WAREHAM
University of Cambridge


Professor John CHAMBERS
Nanyang Technological University


Professor Rudi STOUFFS
National University of Singapore


Professor Ronita BARDHAN
University of Cambridge

SCIENTIFIC UPDATES

Working with agencies to shape the research

Leads

Prof Thomas BURGOINE (CAM)

Assoc Prof Yih Yng NG (NUS)

Asst Prof Bernett LEE (NTU)

Engagement with government agencies and stakeholders in Singapore is a central part of the scientific approach in HD_4. It helps the programme identify policy- and planning-relevant questions, understand what data are available, refine environmental measures, and design studies and analyses that can provide useful evidence for decision-making.

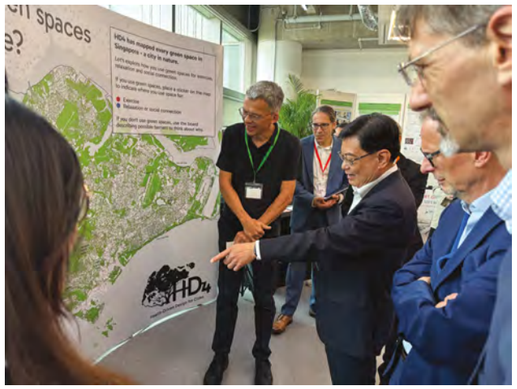
During Q2 and Q3 of 2026, HD_4 strengthened relationships with agencies working across health, food, environmental management, and urban planning. The Singapore Food Agency has provided historical food-outlet records from 2020 to 2026. Discussions with the National Environment Agency, Urban Redevelopment Authority, Health Promotion Board, and town councils have explored agency priorities, the availability of existing data and possible research applications. With the town councils, the team discussed access to sports facilities and tree data. HD_4 and SG100K are working with the Health Promotion Board on the food data needed to implement Intake24 for Singapore.

HD_4 is maintaining its broad network while developing deeper partnerships with selected agencies. Workshops are being arranged to identify a small number of priority questions for the remainder of Phase 1 and the development of Phase 2. These discussions will clarify the evidence required and shape the research questions, analyses, evaluation approaches and possible tools that HD_4 develops.



In June 2026, the HD4 team met the United Nations Development Programme (UNDP) Global Centre Singapore to discuss opportunities for collaboration on air-quality research.

HD_4 had a prominent presence at the National Research Foundation's annual CREATE Symposium in June 2026. Programme Lead Prof Nick WAREHAM (PI, CAM) gave a plenary presentation on healthy ageing and the urban environment. The talk addressed an important priority for Singapore as its population ages and explained HD4's potential to provide evidence about how cities can support health in later life. The wider team presented three scientific posters and an interactive green-space map.



*HD_4 Deputy Programme Lead **Assoc Prof Rudi STOUFFS (PI, NUS)** demonstrated an interactive green-space map to National Research Foundation Chairman Mr Heng Swee Keat at the CREATE Symposium in June 2026.*

The team is contributing a case study on HD4's air-quality work to a forthcoming United Nations Development Programme (UNDP) report on low-cost sensors.

Building a picture of Singapore's urban environment

Leads

Prof Ronita BARDHAN (CAM)

Assoc Prof Rudi STOUFFS (NUS)

Singapore's dense tropical environment exposes people to combinations of humid heat, greenery, transport infrastructure, food outlets and air pollution. HD_4 is developing consistent measures of these conditions from existing agency, satellite and open data, which can be linked with SG100K participants.

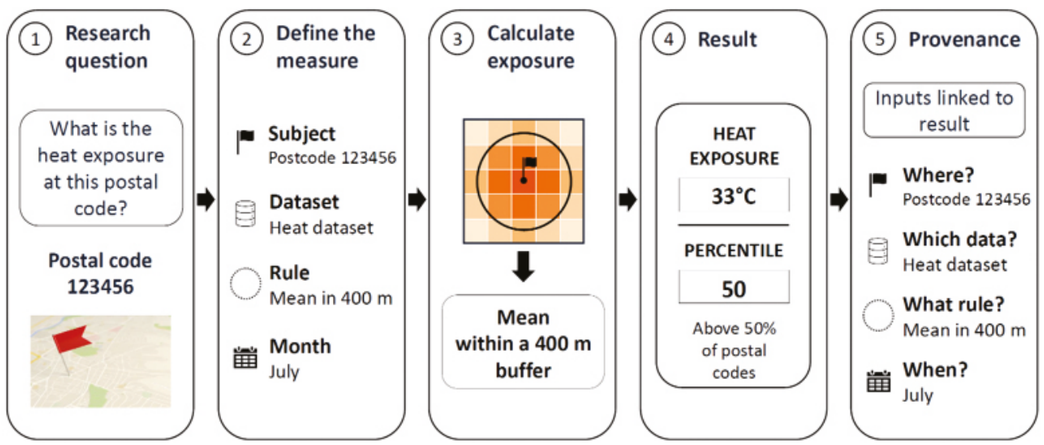
Mapping humid heat across Singapore

Humid heat can place immediate stress on the body, affect people's ability to be physically active outdoors and, with prolonged exposure, contribute to longer-term health risks, making it important for public health and urban planning in Singapore. Between April and September 2026, the team completed a high-resolution dataset based on the Universal Thermal Climate Index and linked it to SG100K. This index combines several weather conditions to estimate how heat is experienced by the human body. The associated method was published in *Sustainable Cities and Society*.

Researchers are developing metre-scale, 24-hour Heat Index maps. This work combines information about Singapore's buildings and vegetation with weather observations. It will allow the programme to examine how humid heat varies across the city and how it relates to behaviour and cardiovascular health. Related work was presented by Yuan WANG (Research Associate, CARES) at the World Sustainable Built Environment Conference in Melbourne in June 2026, showing why land-surface temperature alone may not reflect physiological heat stress.

Making environmental measures consistent and traceable

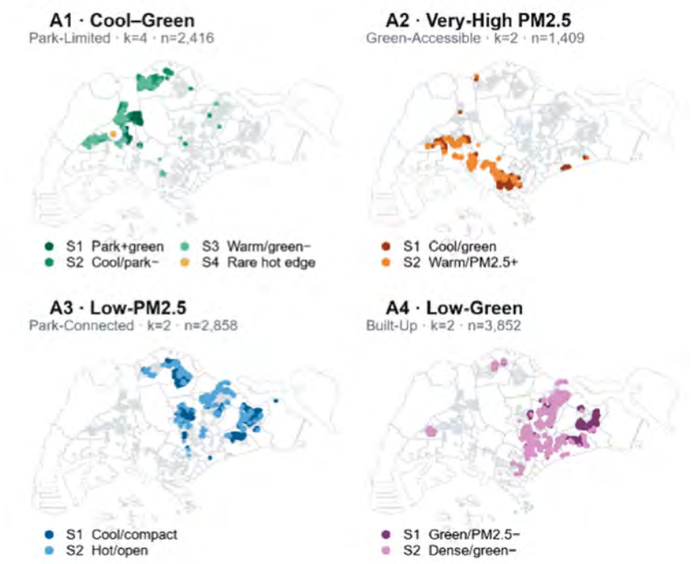
Environmental measures are only useful if researchers can understand exactly what they represent and reproduce them consistently. HD_4 has developed a framework for calculating environmental measures at approximately 120,000 postal-code locations across Singapore. It brings together information on humid heat, greenery, buildings, roads, population, and neighbourhood socioeconomic conditions. For each result, the framework records the source data, period covered, and calculation used. This allows environmental measures to be interpreted, updated and reproduced consistently before they are linked with behavioural and health data. A manuscript describing the framework and its application in Singapore is being prepared.



From a research question to an analysis-ready environmental measure. The framework calculates the exposure for a specified location and records the data and method used. This makes each result traceable and suitable for consistent use in epidemiological analyses. Source: Lee et al., manuscript in preparation.

Understanding combinations of environmental conditions

People experience several features of their environment at the same time, and studying each feature separately may miss how these conditions combine. Researchers used information from five environmental domains to group 10,535 Housing & Development Board (HDB) postal codes into four broad environmental archetypes and ten more detailed subtypes. The archetypes are being prepared for linkage with SG100K and will support analyses that consider combinations of environmental conditions rather than one exposure at a time. The team is examining how these archetypes are distributed across socioeconomic groups as a basis for future research on environmental vulnerability.



Environmental archetypes across 10,535 HDB postal codes. Four broad archetypes and ten more detailed subtypes summarise combinations of environmental conditions across Singapore. They provide a structured way to investigate how multiple exposures relate to behaviour and health.

Understanding the food retail environment

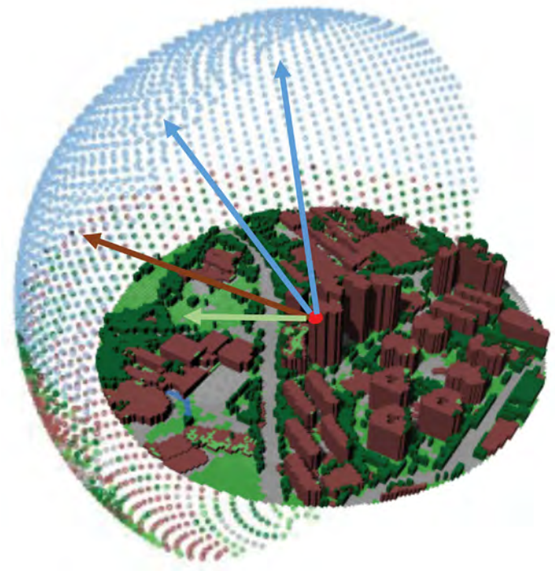
The food outlets available near where people live may shape their food choices and contribute to differences in diet and body weight. Discussions with Singapore agencies have identified consumption of ultra-processed food as an important public health problem. The team has developed preliminary measures of the food-retail environment and has received the historical food-outlet records from the Singapore Food Agency. The records will be processed for analyses of how access to outlets selling ultra-processed foods relates to diet and body weight. Preliminary analyses have examined the distribution of outlets selling ultra-processed foods and how it varies across areas with different socioeconomic characteristics. Dr Lucia SEGOVIA DE LA REVILLA (Research Fellow, CARES) presented the findings at the International Medical Geography Symposium in Toronto in July 2026.

Measuring walking and cycling accessibility

Walking and cycling routes shape whether people can reach parks, sports facilities and daily destinations without a car, influencing their opportunities for physical activity in Singapore's dense tropical environment. Detailed walking and cycling networks have been used to calculate access to parks and sports facilities. These measures have been linked to SG100K and are being refined to include features such as sheltered walkways, gradients, traffic crossings, route stress, surface conditions, and nearby amenities. Connections inside housing blocks are being added to better represent routes through housing estates. Work on the accessibility measures has been accepted for presentation at the International Society for Physical Activity and Health Congress in October 2026. Related research on sheltered walkways has been accepted for Urban Transitions in November 2026.

Measuring greenery

Greenery may support health by providing shade, encouraging physical activity, and improving people's everyday experience of their neighbourhoods. In a dense, high-rise city, the greenery people can see may differ from the amount of vegetation nearby. Researchers have produced annual modelled estimates of visible greenery for 2016 to 2025, covering buildings across Singapore and five building-height categories. Satellite imagery is used to measure the amount and density of greenery around each postal code, while open data sources are used to distinguish different types of green space by their public accessibility and formality. Measures of the physical accessibility of green space are calculated at several walking-distance scales.



How visual greenery is measured. The model traces sightlines from representative points around a building and records whether the first surface seen is vegetation. The measurements are then combined around the building boundary to estimate the greenery visible to residents.

Preparing air-pollution modelling

Air pollution can affect cardiovascular and respiratory health. In Singapore, exposure reflects local sources, shipping emissions, and transboundary pollution. Because pollution varies across space and time, detailed modelling is needed to estimate the exposures experienced by SG100K participants. HD_4 has worked with the National Environment Agency to agree an approach aligned with the agency's existing modelling and needs. Cambridge Environmental Research Consultants will complete the planned three-dimensional air-pollution modelling during Phase 1, including sulphur dioxide. Transboundary pollution, including wildfire smoke, and shipping emissions will be estimated using upwind sensor data through an approach previously used for the agency. The data-sharing request developed jointly by HD_4, the consultants, and the agency is being processed.

How environments relate to health-related behaviours

Leads

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

HD_4 is examining how environmental conditions relate to physical activity, sleep, diet and fitness in Singapore's dense tropical environment. The analyses tested whether greater residential greenery and better walking and cycling access to parks were associated with more physical activity.

An analysis of 38,961 SG100K participants found that greater residential exposure to green space was associated with higher overall and leisure-time physical activity. The amount of green space varied across Singapore and was generally greater among participants of higher socioeconomic status.

A separate analysis used walking and cycling networks to estimate travel time to neighbourhood parks. Better access was associated with a greater likelihood of undertaking at least 600 MET-minutes (a standard measure combining the intensity and duration of activity) of leisure-time physical activity each week. There was little evidence of an association with overall physical activity, which includes activity undertaken for work, transport, and other purposes.

What the early results suggest

The findings indicate that the amount of nearby green space and practical access to parks may both matter for leisure-time physical activity. These observational results identify features that can now be investigated in greater depth.

The sleep analyses tested whether neighbourhood greenery and humid heat were associated with sleep quality. They included 47,971 participants, of whom 43.6% were classified as having poor sleep quality. Poor sleep was more common among women, older participants, Malay and Indian participants, and people of lower socioeconomic status. Preliminary analyses have not found clear evidence that neighbourhood greenery or heat is related to overall sleep quality.

Further analyses will incorporate objective measures of physical activity, sleep and fitness. They will examine the food-retail environment as the required measures become available. Accelerometer data will allow comparison with self-reported activity and analysis of day-of-week and 24-hour patterns. Treadmill tests will provide an objective measure of cardiorespiratory fitness.

Linking environments, behaviours, and health

Leads

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

HD_4 has substantially expanded the data available for examining long-term health. By September 2026, SG100K participants had been linked to electronic health records through the Ministry of Health's TRUST platform, providing detailed information on diagnoses, medications, laboratory measurements, and healthcare encounters. The records can now be analysed alongside the first measures of humid heat, walking and cycling accessibility, and green space.

90,640
participants linked to electronic health records

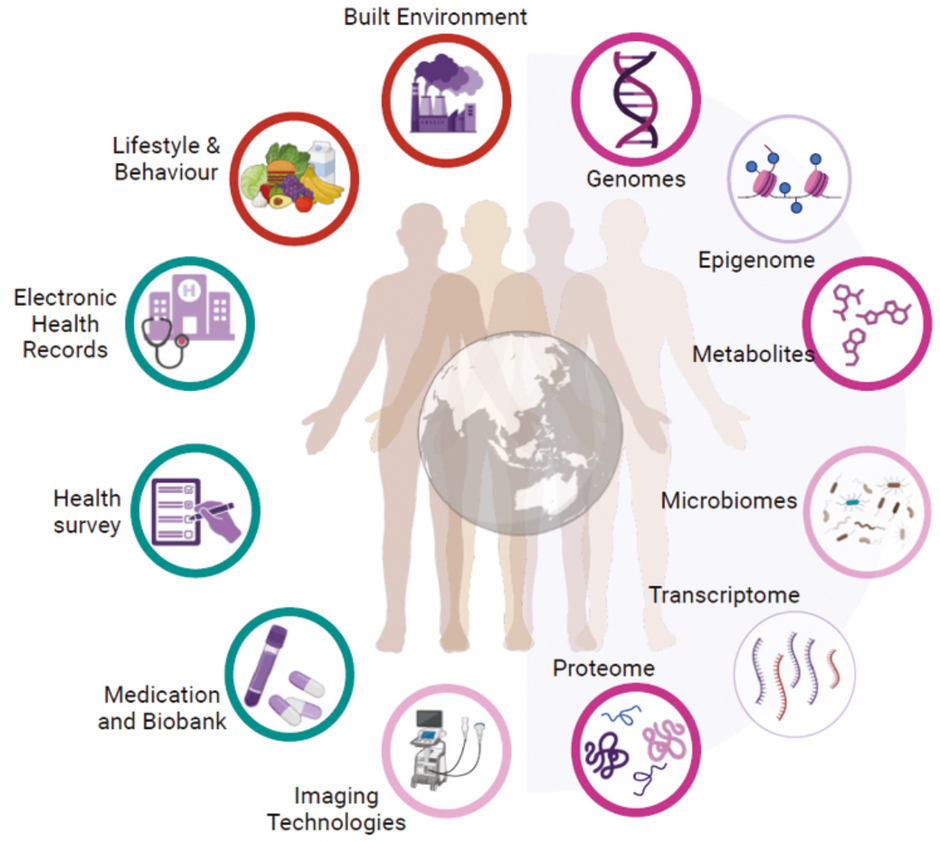
98%
successful linkage rate

3,012
incident cardiovascular events identified to date

The linked records contain a median of 169 diagnoses, 88 medication records and 971 laboratory measurements per participant. This depth of information will allow researchers to study disease trajectories and long-term risk across Singapore's multi-ethnic population.

The analysis tested whether greater exposure to green environments was associated with cardiometabolic health. Early findings suggest that greater exposure is associated with more favourable cardiometabolic profiles across several metabolic traits and measures of metabolic syndrome. These findings are observational and will require further analysis before conclusions can be drawn about cause and effect.

The team tested whether higher diet quality was associated with better glycaemic health, independently of overall and visceral adiposity. Each one-standard-deviation increase in diet quality was cross-sectionally associated with approximately 15% lower odds of prediabetes or previously undiagnosed type 2 diabetes. The pattern was consistent across three established measures of diet quality: the Alternative Healthy Eating Index, the Dietary Approaches to Stop Hypertension score, and the Planetary Health Diet Index. Researchers have established a method for quantifying ultra-processed food intake, providing a basis for future analyses linking diet with the food environment. Dr Ruixin CHI (Research Fellow, NTU) presented these findings at the Singapore Public Health & Occupational Medicine Conference and at ICOMES in Seoul. At ICOMES, Dr Theresia MINA (Senior Research Fellow, NTU) presented related research on dietary risk factors for visceral adiposity.



SG100K brings together information on lifestyle and behaviour, the built environment, electronic health records, health surveys, biological samples and molecular measurements. HD_4 adds detailed environmental exposures to support integrated studies of environments, behaviour and health. Figure created in BioRender by John CHAMBERS (2026).

Measuring people's environments and behaviours in daily life

Leads

Dr Søren BRAGE (CAM)

Assoc Prof Falk MÜLLER-RIEMENSCHNEIDER (NUS)

Assoc Prof Jason Kai Wei LEE (NUS)

A residential address cannot fully describe the environments that people experience as they move through a city. HD_4 is using a set of focused studies to establish which additional assessment methods can be used reliably and at scale within SG100K.

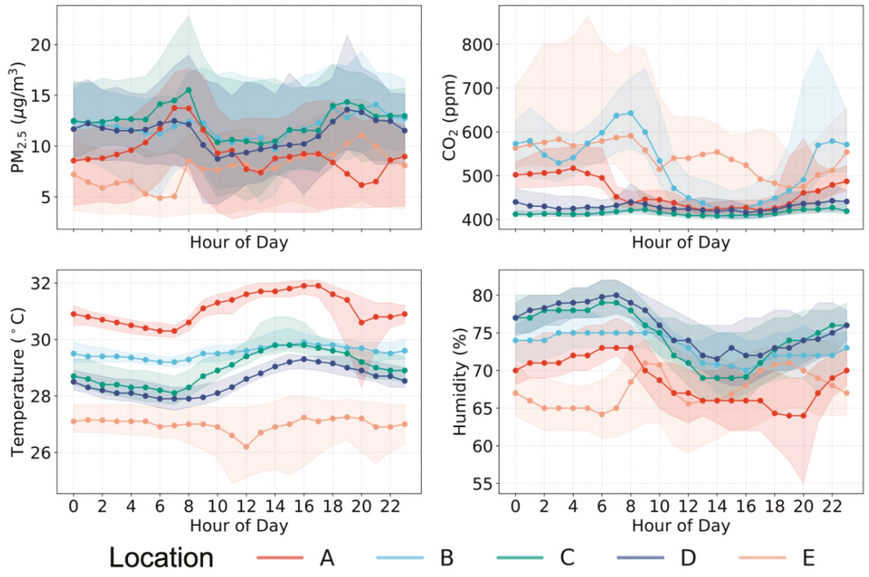
The studies have separate ethics approvals and delivery routes that reflect the safety, governance, and technical requirements of each method.

Fitness and function Supervised in-clinic fitness and physical-function tests have been completed safely, with no issues of concern.	**Diet and dietary behaviours** HD_4 and SG100K are implementing Intake24 for Singapore and are working together on its adaptation, with input from the Health Promotion Board.
Location, movement and travel behaviours Location tracking through BEAM, combined with HD_4's environmental data, will show where participants go and the environments they encounter there.	**Indoor environments** Participants are using consumer-grade sensors in their homes, and dynamic measurements of PM2.5, carbon dioxide, temperature, and humidity are being received.

Four complementary components assess which person-level assessment methods can be used reliably and at scale within SG100K.

HD_4 has established a collaboration with the Behavioural & Environmental digital Activity Monitoring (BEAM) study for location tracking. The collaboration provides an approved data-collection app and established governance and data-integration pathways with SG100K for 12 months of location tracking and access to 12 months of historical phone-based physical activity data. The planned location and historical physical activity data overlap with research-grade accelerometer data already collected in SG100K, allowing the coverage and performance of phone-based measures to be assessed. Combined with the environmental measures described above, location tracking will inform estimates of the exposures participants encounter wherever they go, not only near home, and analyses of their travel behaviour, drawing on HD_4's walking and cycling networks. HD_4 investigators have already developed methods for calculating time-specific exposures from location data.

Building on the earlier analysis of five Singapore homes, participants are now using consumer-grade sensors in their homes, and dynamic measurements of PM2.5, carbon dioxide, temperature, and humidity are being received through the established data pipeline. The data will show how well the equipment and pipeline perform when participants set up the sensors themselves and will inform future indoor-air-quality sampling strategies.



Example data from pre-pilot indoor environment monitoring in five Singapore homes. Sensors captured how PM2.5, carbon dioxide, temperature, and humidity changed over the course of the day. Each colour represents a different home.



Approximate locations of the first participants in the indoor environment monitoring study, shown at the two-digit postal code level. The floors on which the participants live are labelled low (floors 1–9) and medium (floors 10–19); no participants so far live on floor 20 or above. Map data © OpenStreetMap contributors.

Supervised in-clinic fitness and physical-function tests have been completed safely, with no issues of concern. They included a controlled comparison of smartwatch heart rate with chest-based ECG measurements and confirmed a lag in the smartwatch response when activity changed. Establishing the lag under controlled conditions provides a reference for rigorous interpretation and analysis of remotely collected smartwatch data. The tests also generated evidence on exertion and safety-monitoring requirements for possible remote testing. The team is exploring whether heart rate, temperature, barometric pressure, and step data from consumer wearables could eventually support remote assessment of heat stress during daily life.

SHARING HD$_4$'S RESEARCH

HD$_4$ researchers have presented work at events in Singapore and internationally. Further presentations have been accepted for conferences taking place later in 2026.

Conference presentations

- EGU General Assembly, Vienna, May 2026. Dr Mutian MA presented research on remote assessment of health exposures and indoor environments using a low-cost air-quality monitoring system.
- CREATE Symposium, Singapore, June 2026. Prof Nick WAREHAM delivered a plenary presentation on healthy ageing and the urban environment. The wider team presented three scientific posters and an interactive green-space map.
- World Sustainable Built Environment Conference, Melbourne, June 2026. Yuan WANG presented research on the limitations of land-surface temperature for understanding physiological heat stress.
- International Medical Geography Symposium, Toronto, July 2026. Dr Lucia SEGOVIA DE LA REVILLA presented research on historical changes in the number and distribution of Singapore food outlets selling ultra-processed foods.
- Nexus Forum, Oxford, July 2026. Dr Jethro AKROYD gave an invited talk on The World Avatar, featuring work from HD$_4$.
- Singapore Public Health & Occupational Medicine Conference, August 2026, and ICOMES, Seoul, September 2026. Dr Ruixin CHI presented research on diet quality and glycaemic health in a multi-ethnic Asian population.
- ICOMES, Seoul, September 2026. Dr Theresia MINA presented research on dietary risk factors for visceral adiposity using epidemiology, metabolomics and Mendelian randomisation.
- International Society for Physical Activity and Health Congress, Mérida, October 2026. Dr Louise FOLEY has been accepted to present research on measures of access to neighbourhood features that promote physical activity.
- Closing the Air Quality Monitoring Gap Policy Dialogue, Singapore, October 2026. Assoc Prof Rudi STOUFFS and researcher Dr Mutian MA have been invited to give a talk on "Understanding the residential indoor air quality and personal exposures in Singapore" at a joint UNDP-CARES event.
- Urban Transitions, Sitges, November 2026. Research by Dr Thi Anh Hong NGUYEN and Prof James WOODCOCK on the effect of sheltered walkways on active-travel accessibility has been accepted for presentation.

Press and media coverage

In August 2026, *Space Daily* published an article on the cooling effects of urban trees and shade in Singapore. The article discussed research led by Lei XU (Singapore ETH-Centre) and Prof Ronita BARDHAN (PI, CAM), which found that different forms of street shade reduced heat stress across 20 paired sites in Singapore. Shade reduced the Universal Thermal Climate Index by an average of 3.1°C, highlighting the relevance of the environment data collated by HD$_4$ to urban planning and heat mitigation in Singapore.

LOOKING AHEAD

HD4 is now using linked environmental measures, behavioural data and health records in SG100K to examine how Singapore's urban environment relates to behaviour and long-term health. The next stage will deepen these analyses and incorporate food-retail measures, environmental archetypes, air-pollution estimates and location tracking as they become available. Work with Singapore agencies will help identify the questions for which HD4 can provide the most useful evidence for policy, planning and Phase 2. Together, this work will strengthen Singapore's evidence base for designing environments that support healthier lives.

Prof John CHAMBERS

Professor of Cardiovascular Epidemiology (President's Chair)

Lee Kong Chian School of Medicine, Nanyang Technological University

HD$_4$ Programme Lead

Prof Nick WAREHAM

Co-Director Institute of Metabolic Science, University of Cambridge

HD$_4$ Programme Lead



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

Contact: HD$_4$ Knowledge Broker Sharyl Chin, sharyl.chin@cares.cam.ac.uk



PIPS

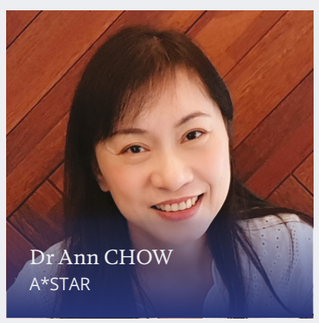
PHARMA INNOVATION PROGRAMME SINGAPORE

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

Project Leads


Professor Dame Lynn GLADDEN
University of Cambridge


Professor Mick MANTLE
University of Cambridge


Dr Ann CHOW
A*STAR

SCIENTIFIC UPDATES

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

The PIPS project commenced in July 2025 led by Dr Ann CHOW (A*STAR), Prof Mick MANTLE (CAM), and Prof Dame Lynn GLADDEN (CAM).

The A*STAR Institute of Sustainability for Chemicals, Energy and Environment (ISCE^2) team continued to perform diffusion, T_1-T_2 and D-T_2 experiments on the Neuros NMR spectrometer, processing the datasets using Python-based data-processing scripts transferred by Prof Mantle from the Cambridge team. These experiments were performed with various solvents, such as methanol, water and acetone, imbibed in an in-house 0.2% Pt/γ-Al_2O_3 catalyst, demonstrating continuity and expansion of the work initiated previously. Figure 3.1 shows T_1-T_2 and D-T_2 correlation plots for methanol imbibed within an in-house 0.2% Pt/γ-Al_2O_3 catalyst, which are in good agreement with the data obtained in Cambridge with the same catalyst. Data processing procedures were also transferred from the Cambridge team to the ISCE^2 team, which led to the generated plots showing only the CH_3 protons in methanol and omitting the faster-relaxing OH protons.

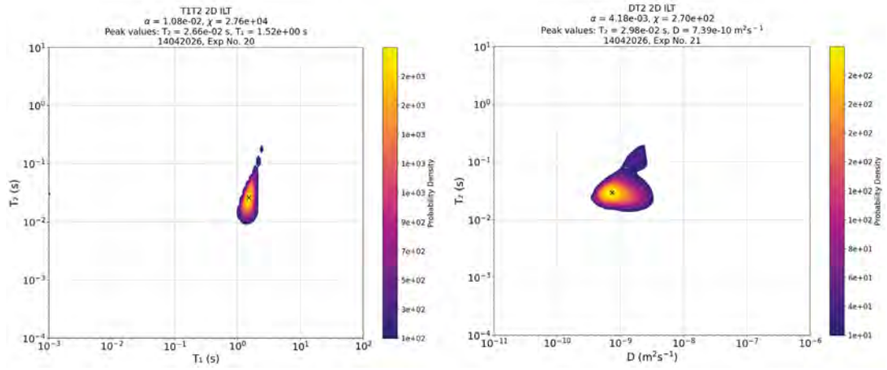


Figure 3.1: T_1-T_2 (left) and D-T_2 (right) distributions of methanol imbibed within an in-house 0.2% Pt/γ-Al_2O_3 catalyst.

Dr Chow and Dr Charmaine Poh from the ISCE^2 team visited Cambridge in July 2026 to meet the Cambridge team and learn to perform imaging experiments on both Topspin and Paravision, as well as solid-state NMR experiments. The imaging experiments were performed on a sample of water imbibed in silica Q30 particles with diameters of 1.7 to 4 mm, which was transported to Singapore and analysed using a spectrometer with an imaging probe at the NTU Centre for High Field NMR. Figure 3.2 shows the T2 mapping data acquired from both the NMR spectrometers in Cambridge and at NTU using the multi-slice multi-echo (MSME) pulse sequence on Paravision, while Figure 3.3 shows the diffusivity maps obtained from the analysis of diffusion mapping experiments at both Cambridge and NTU performed with the DtiStandard pulse program on Paravision. This demonstrated a successful transfer of the imaging and image processing techniques to the ISCE^2 team, giving them the confidence to perform imaging experiments for reaction study in Singapore.

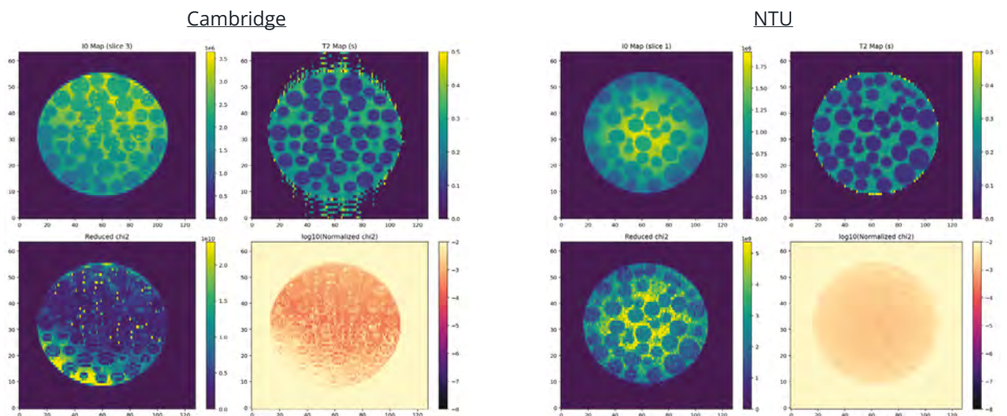


Figure 3.2: Image data obtained with the MSME pulse sequence on water imbibed in silica Q30 particles in Cambridge (left) and NTU (right).

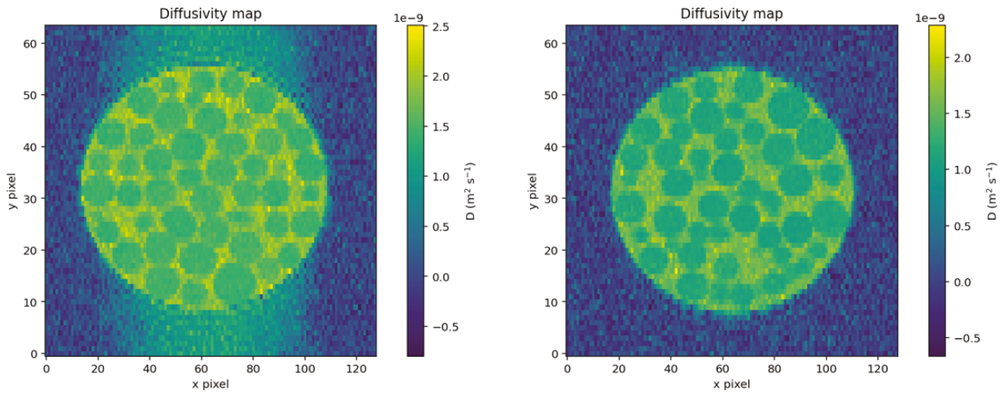


Figure 3.3: Diffusivity maps data obtained with the DtiStandard pulse sequence on water imbibed in silica Q30 particles in Cambridge (left) and NTU (right).

The T_1-T_2 and D-T_2 pulse sequences were also transferred to the NMR spectrometer at NTU used for the above-mentioned imaging experiments. Figure 3.4 shows the D-T_2 distribution of the same sample of water imbibed in silica Q30 particles, with the experiment performed on the NMR spectrometer at NTU. Based on this correlation plot, the T_2 relaxation time of intra-particle water is shorter than that of inter-particle water by an order of magnitude, while the diffusion coefficient D of intra-particle water is slightly smaller than that of inter-particle water. This agrees with the data obtained from the imaging experiments in Figures 3.2 and 3.3.

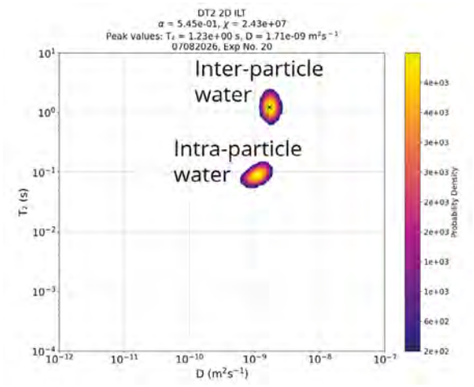


Figure 3.4: D-T_2 distribution of water imbibed in silica Q30 particles.

Finally, as NMR facilities in Singapore do not permit experiments under high-pressure and high-temperature conditions, Dr Jiyuan Fan from the ISCE² team conducted a preliminary study to assess the feasibility of hydrogenating p-chloronitrobenzene (p-CNB) under relatively mild conditions (50 °C and 1 bar). This work was undertaken in preparation for future in situ reaction studies using NMR spectroscopy. For these 20 g-scale batch reactions, 2.5 wt% of *p*-CNB was dissolved in methanol and 0.08 g of an in-house 0.2% Pd/γ-Al_2O_3 catalyst and a Parr reactor were used. Figure 3.5 shows the conversion of p-CNB as a function of reaction time. The results indicate that 52.6% of p-CNB was converted to products after 180 min under the relatively mild reaction conditions of 50 °C and 1 bar. This has given the ISCE² team further confidence to study hydrogenation reactions by NMR using the spectrometers available to them in Singapore.

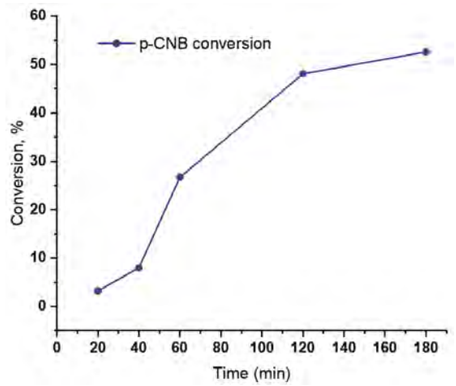


Figure 3.5: Graph of p-CNB conversion against time.

The Cambridge team, consisting of Prof Mantle, Prof Gladden, Prof Andrew Sederman, and Dr Andrew YORK (PDRA), have made significant progress during the period April to September 2026. Dr York completed his onboarding and began familiarising himself with the T_1-T_2, D-T_2 NMR pulse sequences used to investigate reactant/solvent interactions with carbon-based catalysts. Initial NMR/MRI experiments were performed using Kureha SP A-BAC 200 mm spherical carbon support particles. However, following discussions with industrial partners, the team decided to switch to GL sciences carbon support particles with a diameter 400 mm for subsequent NMR/MRI experiments.

New 2D chemically selective multislice-multiecho (MSME) ^{1}H MRI pulse sequences were developed in Cambridge to selectively image both inter- and intra-particle liquid (methanol) species in a 12 mm i.d. glass cold flow micro trickle bed reactor (mTBR). Figure 3.6 shows 5 1 mm-thick horizontal (xy) slices taken at 3.5 mm vertical intervals down the mTBR with an in-plane pixel resolution of 163 mm.

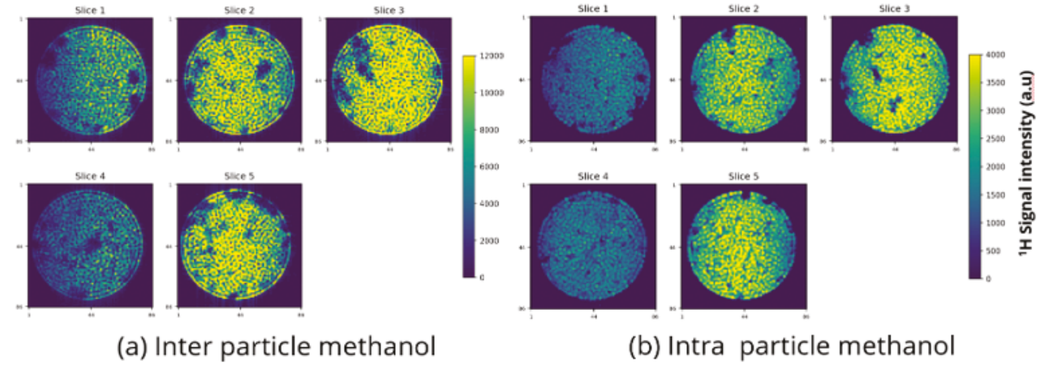


Figure 3.6: ^{1}H 2D MSME chemically selective images of a micro trickle bead reactor packed with GL sciences 400 mm spherical carbon support materials, flooded with methanol. (a) inter-particle methanol and (b) intra-particle methanol. Field of view in xy-plane is 14 mm × 14 mm, data matrix size 86 × 86; 1mm slice thickness; in-plane pixel resolution of 163 mm.

In addition to showing both inter- and intra-particle methanol, Figure 3.6 shows air bubbles as dark patches in the images. The mTBR flooding protocol has since been modified to ensure that the reactor can be fully flooded without trapping air bubbles. During this reporting period, work has focused on studying cold-flow hydrodynamics in an mTBR using the chemically selective 2D MSME ^{1}H MRI pulse sequence to acquire images during gas(air) and liquid(methanol) flow. A significant amount of time has also been devoted to developing Python image-analysis algorithms to process the raw MRI data and produce images of the gas and liquid fractions during multiphase flow. Figure 3.7 shows two sets of images acquired at different times from an mTBR fully flooded with methanol in the absence of liquid flow.

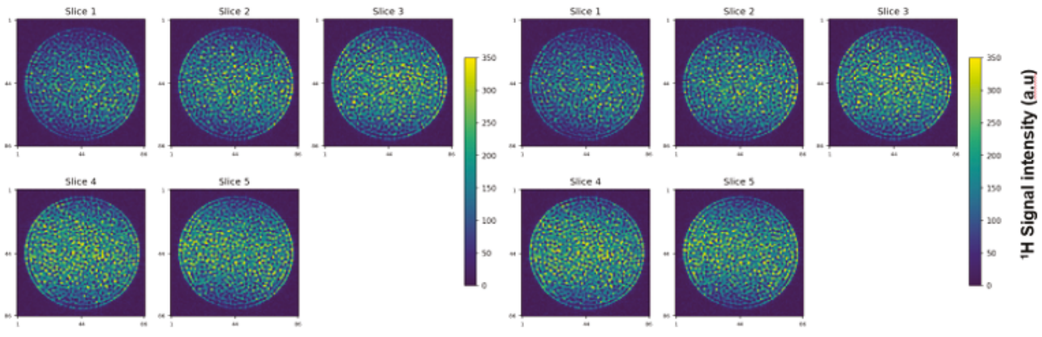


Figure 3.7: ^{1}H 2D interparticle chemically selective MSME images taken at (a) t = 0 min and (b) t = 180 mins after flooding the mTBR with methanol. 1 mm slice thickness with an in-plane pixel resolution of 163 mm.

The images shown in Figure 3.7 can be used as reference images to create a "division" map of a fully liquid-flooded mTBR. Images of a "dry" mTBR, from which the inter-particle liquid has been removed by flowing gas through the reactor, can also be used to create a reference map of gas-only regions, where the signal represents noise. Figure 3.8 illustrates this process, with the liquid-flooded regions shown in yellow and the dry(noise) regions shown in dark blue.

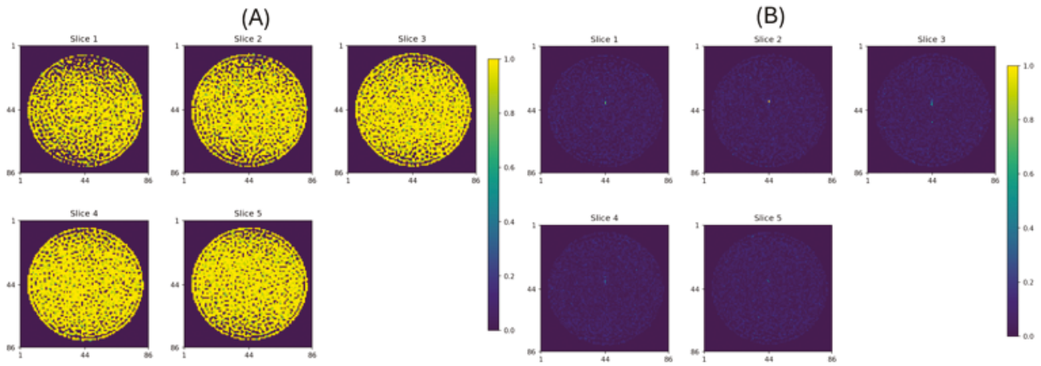


Figure 3.8: ^{1}H 2D interparticle chemically selective MSME images created from: (A) the division of the two images shown in Figure 3.7 taken at t = 0 min and t = 180 min; (B) the result from the division of a "dry" mTBR by the reference image shown in Figure 3.8A.

The pixel intensities from the images shown in Figure 3.8 can then be plotted as a histogram, allowing the ^{1}H signal intensity to be objectively partitioned into three categories: gas-only, liquid-only and mixed gas–liquid regions (Figure 3.9). The 97.5th percentile is used to identify gas-only regions, while the 2.5th percentile is used to identify liquid-only regions. Pixel intensities between these two thresholds are assigned to mixed gas–liquid regions.

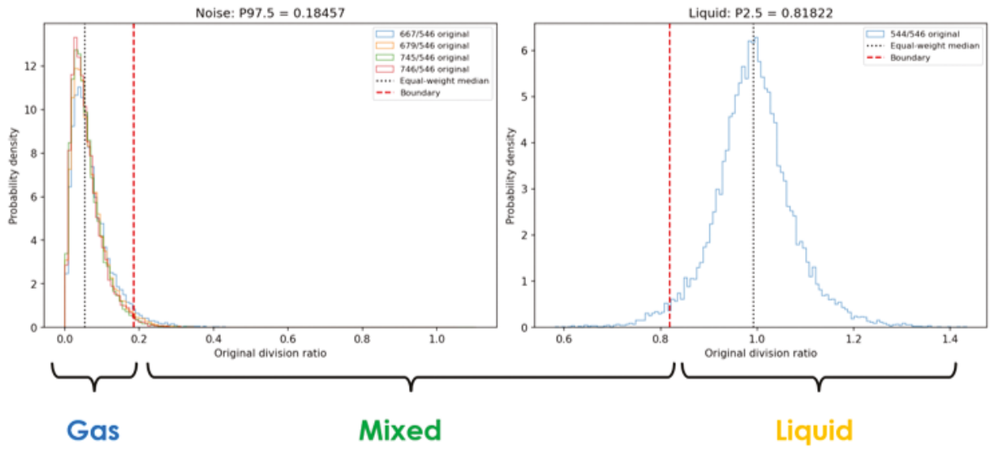


*Figure 3.9: Histogram of pixel intensities from Figure 3.8, showing the partitioning values (red dashed lines) for Gas, **Mixed** and **Liquid** regions used for the segmentation of multiphase flow images.*

The partitioning values are then used to segment the raw gas-liquid flow images into 3 different regions containing gas only, mixed gas-liquid, and liquid only fractions as shown in Figure 3.10.

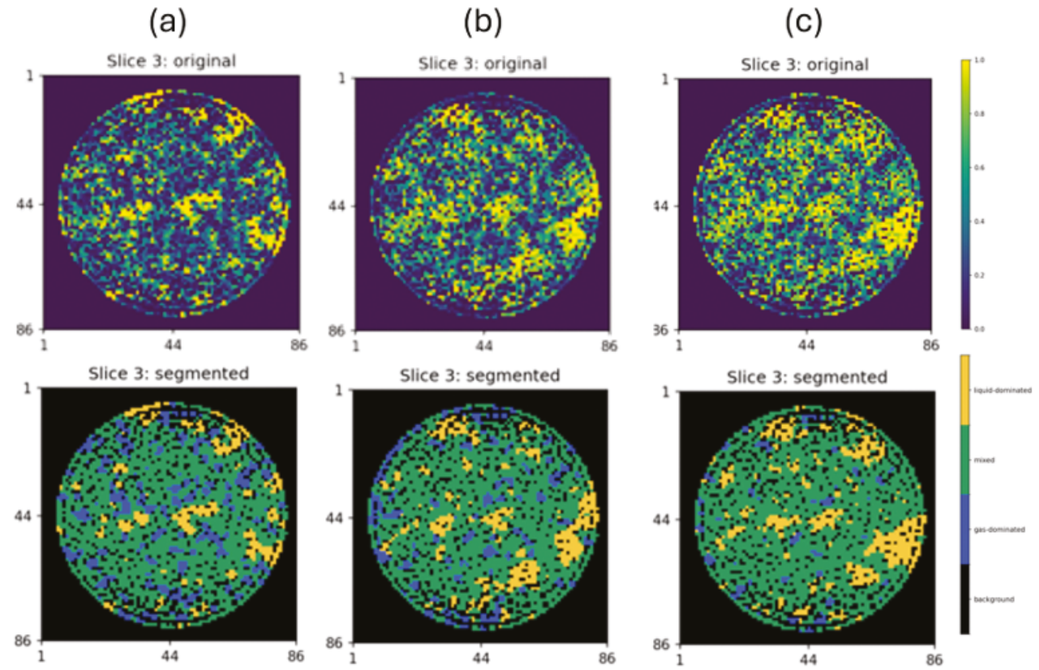


Figure 3.10: Original multiphase flow ^{1}H 2D MSME images and segmented MR images for slice 3 (middle of mTBR) taken during gas and liquid flow, for a constant gas (air) flow rate of 2.0 ml min^{-1} and three different liquid flow rates: (a) 1.0 ml min^{-1}; (b) 2.7 ml min^{-1}; (c) 4.0 ml min^{-1}. The segmented data uses the histogram partitioning data shown in Figure 3.9.

This analysis process is then repeated for many images taken at different gas-liquid flow rates. Figure 3.11 shows the overall results for a series of experiments where the gas flow was kept constant at 2.0 ml min^{-1} and the liquid flowrate was varied from 1, 2 to 4 ml min^{-1}.

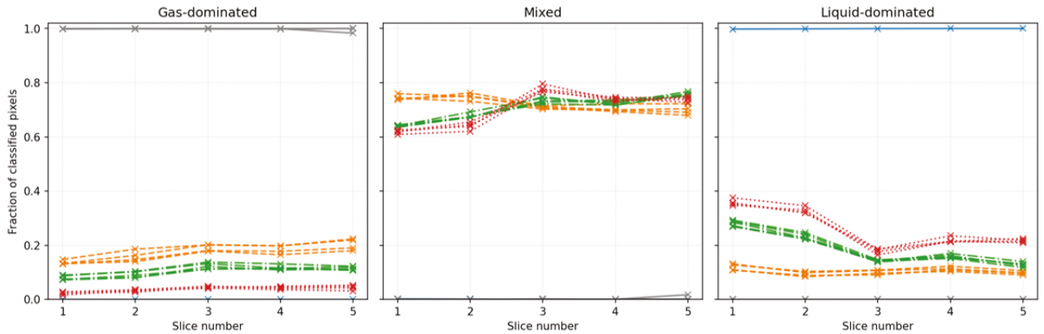


Figure 3.11: Plots showing the gas-dominated, mixed gas-liquid and liquid dominated fractions from 5 different slices taken during a multiphase gas-liquid flow experiment of constant gas flow (2.0 ml min^{-1}) and three different liquid flowrates: 1.0 (orange), 2.7 (green) and 4.0 (red) ml min^{-1}. Note grey and blue symbols are for pure gas (noise) and pure liquid images respectively.

Figure 3.11 demonstrates good reproducibility across the three liquid flow rates. The liquid fraction increases with increasing liquid flow rate, accompanied by a corresponding decrease in the mixed gas–liquid fraction. The gas-dominated regions remain reasonably constant across the different liquid flow rates.

In addition to the hydrodynamic studies, the Cambridge team has been using 2D NMR exchange spectroscopy to investigate liquid mass transfer within the mTBR and conducting liquid-velocity imaging in the cold-flow mTBR. This work is ongoing. The team has also finalised and submitted the design of an in situ NMR/MRI chemical micro trickle-bed reactor made from PEEK. This reactor will be used to study the hydrogenation and debenzylation reactions described in the original proposal and to conduct hydrodynamic studies under hydrogenation conditions.

Other Projects

CARES-FUNDED PROJECTS

LCER PHASE 2

Low-Carbon Energy Research

Dr B. HARIKRISHNAN (Research Fellow, CARES) has been working on the application of the low-order Incompletely Stirred Reactor Network (ISRN) model for a laboratory-scale high-pressure partially cracked ammonia combustor. Validation is performed against the experimental data of SINTEF burner. The required mixing field statistics are obtained by performing Large Eddy Simulation – Conditional Moment Closure (LES-CMC) simulations at two reference conditions of ammonia decomposition ratios: 0.25 (10 bar) and 0.50 (5 bar).

Figure 4.1 shows fields obtained from ISRN with the mixture fraction and its sub-grid scale variance. The temperature field shows increased flammability due to the increased presence of hydrogen mass fraction in the fuel composition. Also, its NOx results are compared against the LES-CMC for decomposition ratios 0.5 and 0.9. Though the ISRN uses the 0.50 case as the anchor point, it was able to make valid predictions for a case far from the reference conditions.

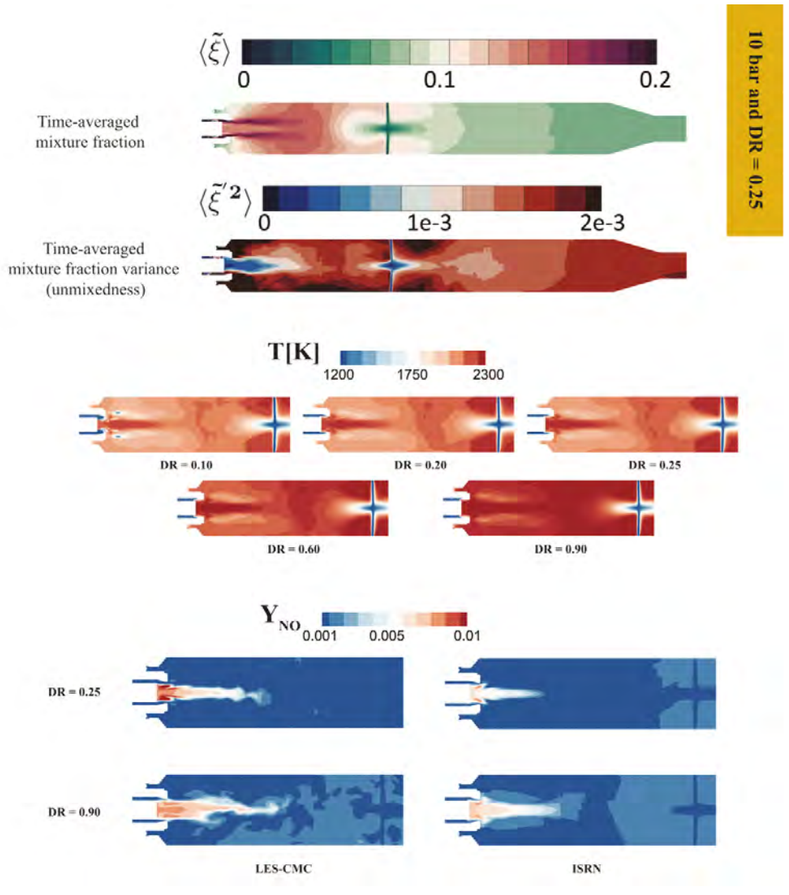


Figure 4.1: Mixing field statistics and ISRN simulations performed using DR=0.25 and 10 bar pressure as the anchor point.

Figure 4.2 shows the statistics for the case with decomposition ratio 0.5 and 5 bar pressure. It also includes the ISRN predictions for NO mass fractions. The primary zone NO production is high due to the stoichiometric condition, and it drops with the increase in the decomposition ratio.

Figure 4.3 shows the exit NOx results for both pressure cases compared against the LES-CMC and the experimental results. ISRN demonstrates its ability to predict the NOx trends. Also, the trend was recoverable regardless of the underlying reference CFD case. Additionally, the ability to switch the underlying mechanism made ISRN ubiquitous for the design engineers of the next-generation gas turbines.

Current progress includes the development of the CFD solver agnostic ISRN solver. It was further applied to the primary stage of the industrial burner of Siemens Energy. Future direction will focus on performing extensive operating condition exploration for optimal exit NOx.

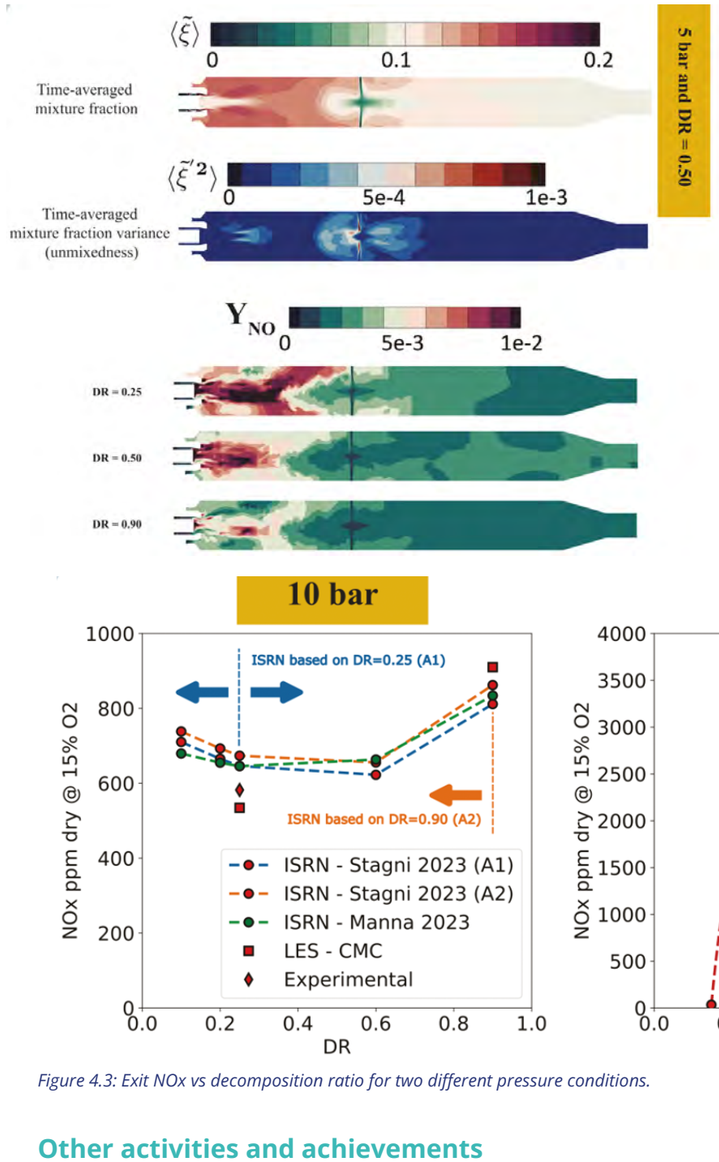


Figure 4.2: Mixing field statistics and ISRN simulations performed using DR=0.50 and 5 bar pressure as the anchor point.

Figure 4.3: Exit NOx vs decomposition ratio for two different pressure conditions.

Other activities and achievements

Dr B. HARIKRISHNAN (Research Fellow, CARES presented "Modelling Emissions from Ammonia Combustors with the Incompletely Stirred Reactor Network method" at the 41st International Symposium on Combustion in Kyoto, Japan from 26 – 31 July 2026.

NH3-SOFC

Decarbonization with Green Ammonia Using Solid Oxide Fuel Cell (SOFC) for Power Generation

Dr Xingyu CAO (Research Fellow, CARES) has been developing and analysing a multiphysics model of a tubular ammonia-fuelled solid oxide fuel cell (NH_3-SOFC). During this reporting period, sensitivity analyses were carried out to investigate how operating conditions, electrochemical kinetics, material properties and transport parameters influence key model outputs, including current density and ammonia conversion. The analysis identified the parameters with the greatest influence on the predicted cell performance and showed that their relative importance varies across different operating conditions, reflecting a combination of kinetic, transport and material effects. The modelling and sensitivity-analysis framework was also applied in a related master student research project to compare sensitivity results obtained under different modelling conditions. More recently, preliminary work has begun to extend the NH_3-SOFC model towards mixed-fuel operation.

Other activities and achievements

Dr Cao presented "Multiphysics Modelling of Ammonia Solid Oxide Fuel Cell for Design Optimisation" at the Great Western Electrochemistry Meeting on 8 June 2026 at the University of Bath, UK.

ECO2RR

Development of Advanced Catalysts for Electrochemical Carbon Abatement

Dr Chencheng DAI (Senior Research Fellow, CARES) has studied the cost-effective electrochemical ethanol oxidation reaction (EOR) on Pt-based catalysts in acidic medium as a potential anode reaction coupled with CO_2 reduction or hydrogen cogeneration. Some of the Lewis-acidic oxides such as SnO_2 and WO_3 are well-known for enhancing alcohol oxidation under alkaline conditions, where their hydroxylated surfaces and interactions with hydroxide ions facilitate the alcohol deprotonation on Pt surface. However, these effects can be diminished because of changes in surface protonation and hydroxyl availability, whereas oxides such as CeO_2 and Ta_2O_5 may retain promotional effects through additional redox, oxygen-vacancy, water activation or strong oxophilic interactions. The PtRu is know for high activity towards alcohol oxidation catalysis, especially after the Pt-Ru surface reconstruction via pretreatment. Therefore, when metal oxides are incorporated into carbon-supported PtRu catalysts, they may influence not only the intrinsic catalytic chemistry but also the activation process. The oxide-to-carbon ratio is therefore expected to have an optimum range.

Other activities and achievements

Dr Dai presented a poster "Development of on-site, on-demand ammonia-to-hydrogen e-cracking bench-top chemical mini-factory" at the Urban Solutions and Sustainability R&I Congress from 5 - 6 February 2026 in Singapore.

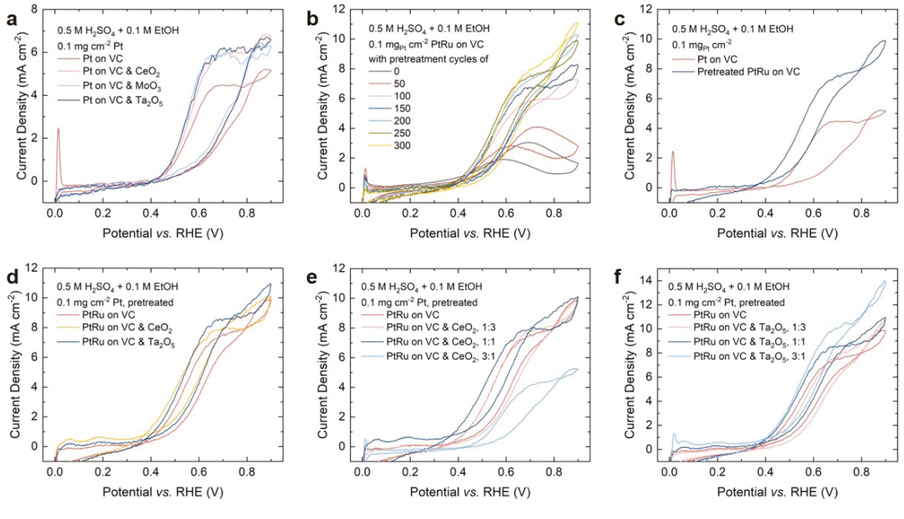


Figure 4.4: (a) Cyclic voltammetry (CV) curves of EOR on Pt with various metal oxide substrates. (b) CV curves of EOR on PtRu with different pretreatment scans. (c) CV curves of EOR on optimized PtRu and Pt catalysts. (d) CV curves of EOR on PtRu with various metal oxides catalysts. (e&f) CV curves of EOR on PtRu with substrates of different oxide-to-carbon ratios.

Publications

ALL PUBLICATIONS WITH CREATE ACKNOWLEDGEMENT

Newly added publications for this reporting period are coloured in red. For a full record of earlier publications, please visit the CARES website and navigate to the "Publications" tab

Centre for Lifelong Learning and Individualised Cognition (CLIC)

Feng, Shengchuang, Nadhilla Melia, Akshay Abraham, et al. 2026. 'QualGames: A Qualtrics Implementation and a Database of Behavioral Game Theory Tasks'. *Behavior Research Methods* 58 (8): 219. https://doi.org/10.3758/s13428-026-03081-2.

Feng, Shengchuang, Nadhilla Melia, Hui Shan Yap, et al. 2026. 'Over Fifteen Years of Confusion: How the Big Five Inventory Mismeasures Openness'. *European Journal of Personality*, May 22, 08902070261450714. https://doi.org/10.1177/08902070261450714.

Fischer, Nastassja L., Kastoori Kalaivanan, Ke Tong, et al. 2026. 'Set-Shifting and Task-Switching Make Differential Contributions to Divergent Thinking in Adolescence'. *BMC Psychology* 14 (1): 733. https://doi.org/10.1186/s40359-026-04584-5.

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

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