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Smarter Pathways to Energy Transition

Centre for Multiscale Energy Systems (CMES)

Our focus

Few global challenges are more pressing than moving from 20th-century energy technology to 21st-century energy systems. Energy systems across all sectors need to shift sustainably from carbon-intensive fossil fuels to a diverse mix of energy sources, where renewables play a central role. The synergy of distributed and concentrated forms of both renewable and non-renewable energies is a key factor underpinning Australia's advantages in the global energy transition. The performance of future energy systems must rely on innovations at both elementary and systemic levels. As a leading university in energy transition, the University of Queensland (UQ) provides a multidisciplinary ecosystem of expertise and unique capabilities in multiscale systemic modelling of complex systems, offering a robust, technically sound, and clear picture of our energy choices today and in the future.

The Centre for Multiscale Energy Systems brings together UQ's energy research expertise. A dedicated team of over 30 researchers across the engineering faculty and science disciplines, along with more than 20 PhD students, works in close collaboration with industry, academia, and governments.

Driven by our strong collaborations within UQ and worldwide, our research spans energy conversions and storage, various thermofluid applications, materials for renewable hydrogen storage and utilisation, design, systems analysis, as well as Australia's role in the world's power generation.

Thermodynamic power cycles

The central question of an energy system is always how effectively heat from any source is converted to useable power. This is what a heat engine does. In the traditional fossil-based energy era, steam cycles and reciprocal internal combustion engines play a dominant role. Future energy, however, moves towards more diverse energy sources. The demands for more efficient, flexible, and sustainable power conversion technologies are more emergent than ever.

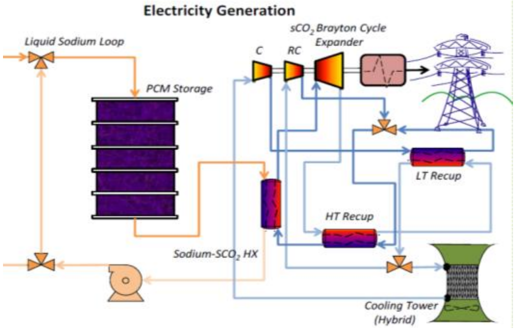
As a core area, CMES has committed to the development and commercialisation of the next-generation power cycle technologies for over a decade. Our primary focus includes supercritical CO2 and organic Rankine (ORC) cycles, aiming at applications including but not limited to renewable and clean power generations, propulsion, and waste heat recovery.

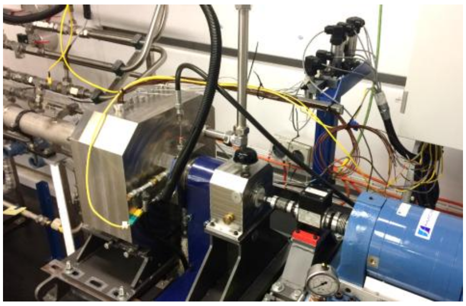
Highly efficient and compact power conversion cycles with flexibility in adaption are sought after in the current transition to decarbonisation. sCO2 cycles have great advantages over steam cycles in terms of efficiency, compactness, responsiveness, and quietness. Their potential is convincing and widely recognised in waste heat utilisations, renewable thermal power, and next generation nuclear energy.

CMES established expertise and capacities in designs, modelling, tests, optimisations, and lab-scale demonstrations of complete sCO2 cycles and ORCs as well as their specific components. The Centre processes world-class facilities including a test loop for high-pressure, temperature sCO2 and organic fluid radial turbine cycle, 1 MW heaters, refrigeration chillers, and a modular low-temperature ORC. Previous applications of these capacities and facilities in major research programs include the Queensland Geothermal Energy Research and the Australian Solar Thermal Research Institute (ASTRI).

Direction key personnel

- **Dr Yuanshen Lu**
- **Emeritus Professor Hal Gurgenci**
- **Prof Stephen Wilson**





Figures from top to bottom:
- *The high-pressure sCO2 turbine loop test facility*
- *Power block designs for concentrated solar thermal plant*
- *The 7 kW organic fluid radial turbine assembly*
- *The rotor of the radial turbine designed in CMES*

Solar and wind energy

Analysis of wind flow in renewable energy applications, including solar thermal power plants, solar farms, urban photovoltaics, agrivoltaics, and wind turbine farms, and its impacts on cooling, wind loading, power generation efficiency, and the surrounding environment to inform design and operational strategies.

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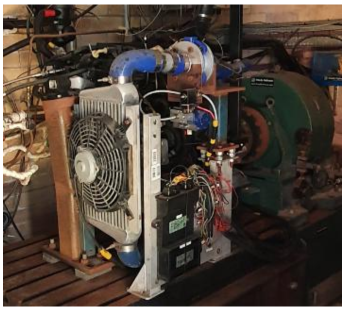
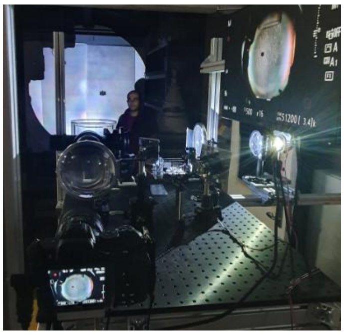
Thermo-fluids and combustion

Over the past 15 years, CMES have gained international reputation in heat transfer, cooling, and combustion. Remarkable achievements include but are not limited to natural draft dry cooling towers (NDDCTs), air-cooled heat exchangers, evaporative pre-cooling technologies, combustion models, etc. The Centre has created the novel concept of small scale modular NDDCTs for a variety of cooling applications such as coal seam gas industry. The concept brings flexibility and cost-effectiveness on top of the intrinsic advantages of NDDCTs. As a demonstration of the concept, the Gatton NDDCT is the only facility of this kind in Australia capable of a range of cooling tests. Gatton NDDCT is 20 m tall and equips with 18 plate fin-tube heat exchanger bundles with a total cooling capacity around1.5 MWth.

Direction key personnel

- **A/Prof Alex Klimenko**
- **Dr Yuanshen Lu**





One of the key capabilities of CMES is research in fundamental combustion and heat transfer. Our goal is to build a deep understanding of the multi-physics in thermal and species transportations and thermo-fluid interactions with physical structures (e.g., porous media). CMES researchers and their colleagues in the School of Mechanical and Mining Engineering have proven expertise in sophisticated experiments and advanced modelling:

- Design and building of research infrastructures and instrumentation, e.g., wind tunnels and ICE test facility, for a wide range of thermo-fluids tests.
- Advanced measurement and flow visualisation techniques, including particle image velocimetry (PIV), laser Doppler analyser (LDA), PDPA, and Schlieren imaging, to study complex flow problems such as boundary layers and wake of heat exchanger tubes, water sprays from nozzles, plume of thermal stacks, etc.
- computational fluid dynamics tools to model complex thermo-fluids properties and behaviours in natural convection & convective heat transfer, spray and atomisation, evaporation.

Figures from top to bottom:

- *The Gatton NDDCT facility*
- *The heat exchanger panels in the Gatton NDDCT*
- *Spray of saline water for evaporative cooling*
- *Metal foam heat exchangers tested in 45-101 Wind Tunnel*
- *A novel retroreflective background Schlieren facility*

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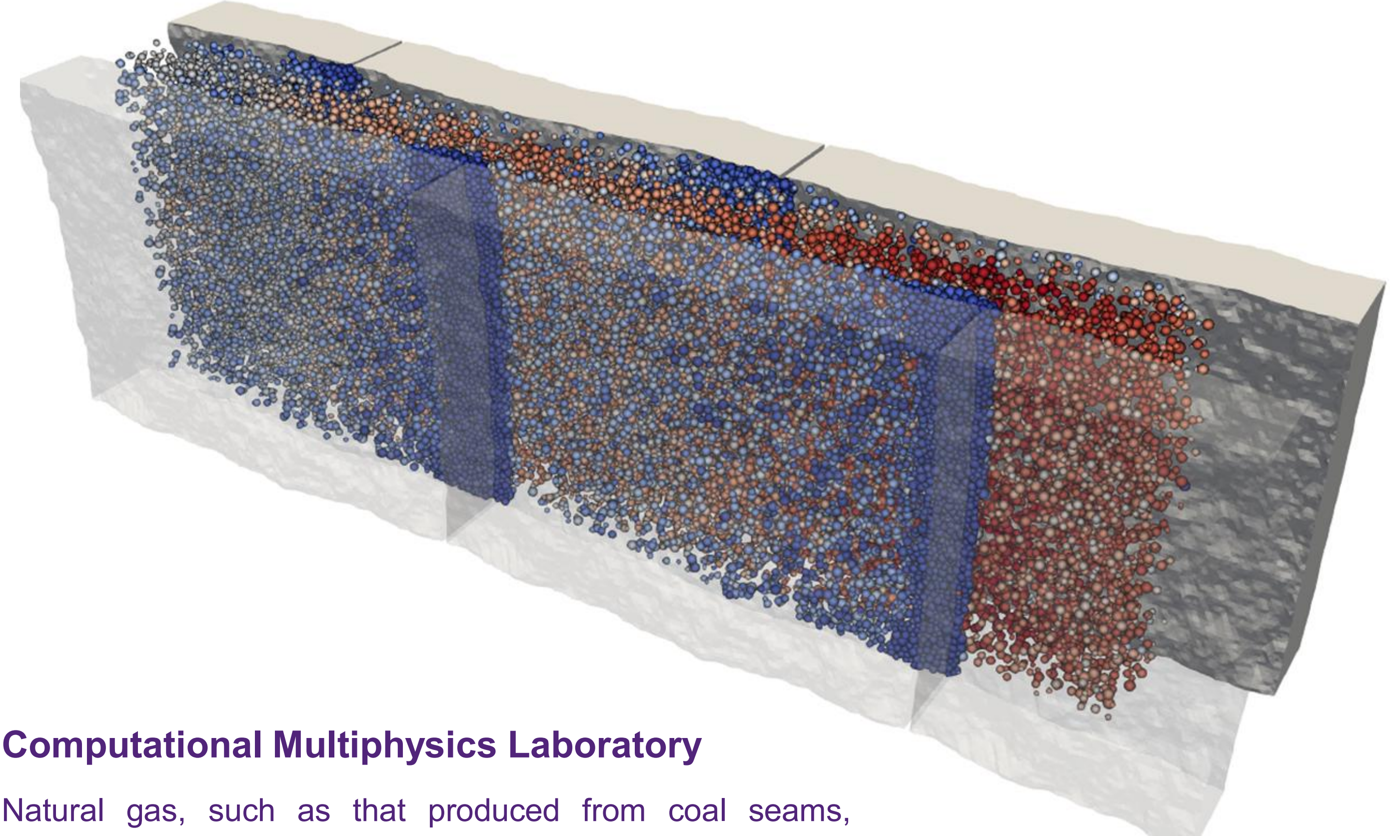


Computational Multiphysics Laboratory

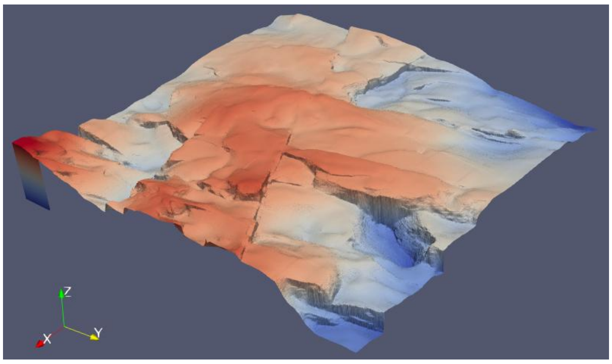
Natural gas, such as that produced from coal seams, remains an integral component of the nation’s plans for net zero carbon emissions by 2050. It will support the deeper penetration of renewables into the electricity market and play a role in manufacturing and hydrogen production. The ongoing availability of gas requires the maximisation of production from available resources and the minimisation of impacts on stakeholders and the environment.

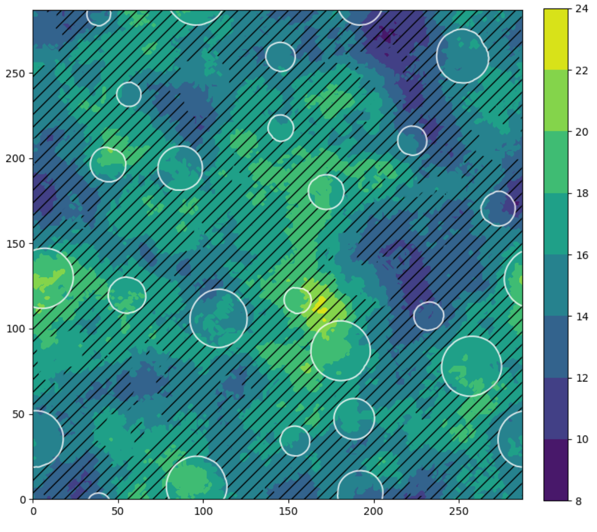
The Computational Multiphysics Laboratory (CML) within CMES has developed computational tools for the prediction of complex multiphase flows associated with unconventional gas production, with a focus on the coal seam gas (CSG) industry. These tools unify the benefits of the lattice Boltzmann (LBM), finite element (FEM), and discrete element methods (DEM) to predict the interaction of fluids, solids, and particles, respectively. Deployment on world-class HPC infrastructure facilitates high-fidelity predictions of phenomena at industry-relevant scales.

Working with industry partners including Origin Energy, Arrow Energy, and Santos, the CML has solved problems related to proppant transport in hydraulic fractures, co-mingled water and gas flow during CSG production, and surface movement induced by CSG activity. For example, proppant transport modelling has been used to quantify the performance of non-traditional particles and the effect of electrostatic interactions on microproppants. Two-phase flow simulations have generated new insight on the relative permeability of coal cleats and fractures. Lastly, coupling of flow with geomechanics has been used to provide guidance to government on the potential magnitude of CSG-induced surface movement and its impact on landholders.

Direction key personnel

- **A/Prof Christopher Leonardi**
- **Dr Travis Mitchell**





Figures from top to bottom:

- *LBM-DEM simulation of proppant injection in a coal fracture and branching cleats*
- *Digital optical microscopic image of a coal cleat, used to inform simulated fractures*
- *Distribution of water (hatched) and gas in a rough fracture with varying aperture*

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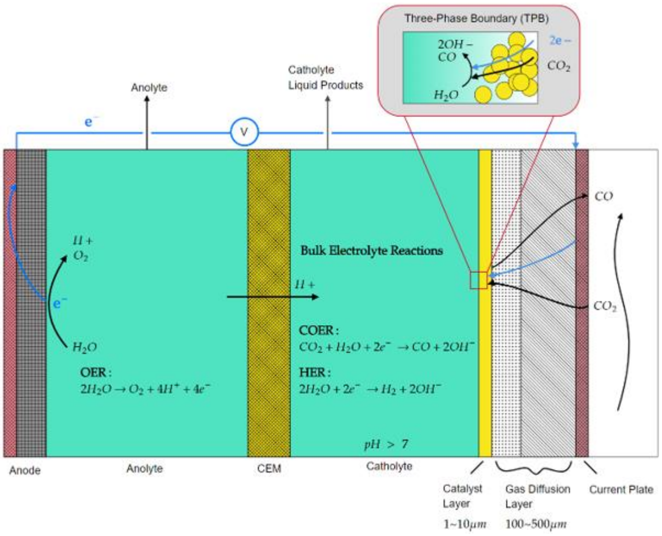
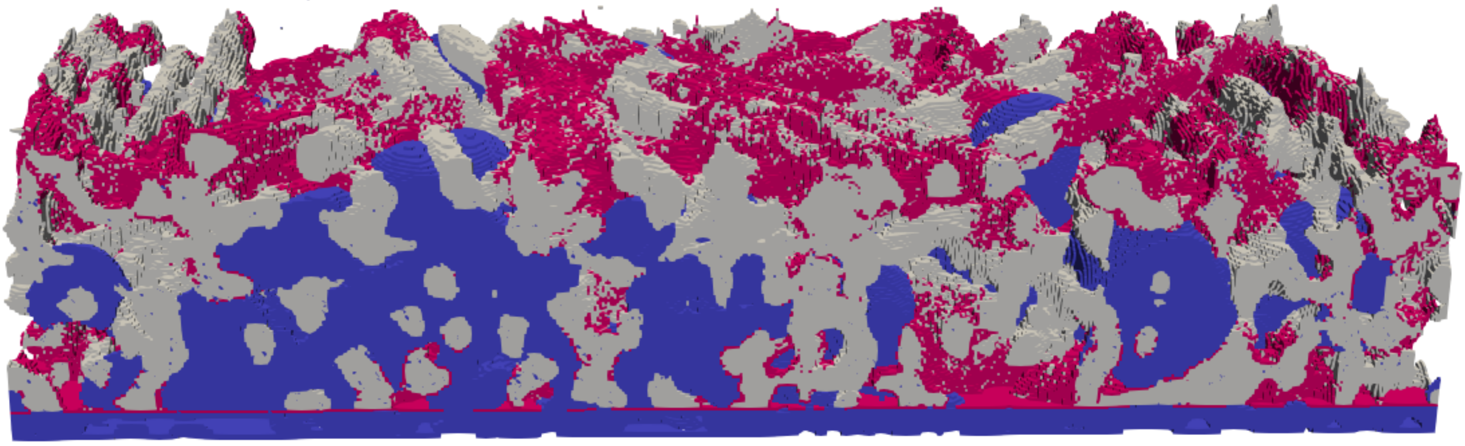
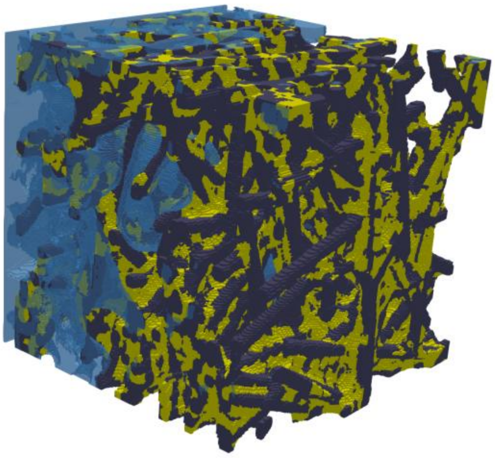
The Computational Multiphysics Laboratory (CML) within the CMES leverages its capability in high-fidelity numerical modelling to understand the failure mechanisms of gas diffusion electrodes (GDEs) in electrochemical devices. This research focuses on CO_2 electrolysers to provide a pathway for utilisation of carbon dioxide. This technology seeks to provide a sustainable pathway to produce various chemicals and fuels while mitigating anthropogenic greenhouse gas emissions. The electrolyser technology relies on efficient and reliable GDEs to facilitate the electrochemical reduction of CO_2 to targeted products to serve as carbon-neutral feedstocks for the chemical production industry or as scalable energy storage.







This technology currently lacks the required durability to operate at scale with early onset of failure limiting its commercial viability. State-of-the-art GDE designs are based on repurposed proton exchange membrane fuel cell (PEMFC) materials, which embody many desirable properties, but do not meet all the necessary requirements for longevity. GDEs have complex, multi-scale porosity that facilitates multiphase interactions and chemical reactions. When scaling up CO_2 electrolysers, the GDEs tend to fail due to two primary modes:

1. Flooding, where the electrolyte permeates into the GDE inhibiting transport of CO_2 to reaction sites;
2. Carbonate precipitation, where the formation of low-solubility carbonates promotes both flooding and precipitation, blocking transport of CO_2.

The **CML makes use** of experimental imaging, synthetic generation of stochastic materials, and high-fidelity multiphase simulations to elucidate the fundamental, pore-scale effects that lead to these modes of failure. This research aims to develop novel electrode materials and structures that are sufficiently resilient to enable the scale up of CO_2 electrolysis devices, as well as improve our understanding associated with GDEs applied in a variety of electrochemical systems.

Figures from top to bottom:

- *Schematic of a CO2 electrolysis cell indicating the various components with a focus on the three-phase interaction point in the cathode where the desired reaction occurs.*
- *Study of breakthrough time for electrolyte penetrating cracks a microporous layer and propagating through the structural support in the form of a gas diffusion layer. Geometry was obtained from existing literature using micro-CT imaging.*
- *Study of electrolyte breakthrough time in a stochastically generated, mixed-wet gas diffusion layer to study the influence of PTFE content and distribution.*

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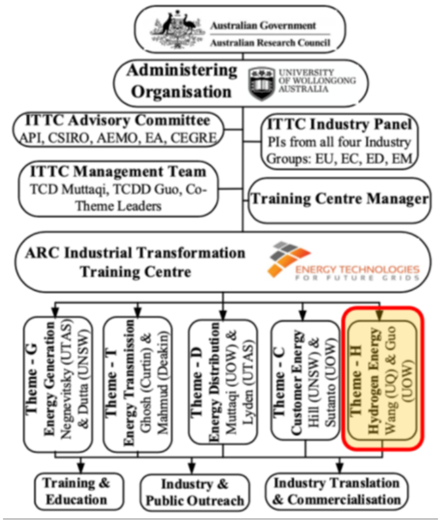
Cast Mg Alloys for Hydrogen storage

Innovative H_2 energy storage and utilisation technologies are required to support Australia’s industrial-scale clean H_2 production capabilities and increase H_2 power generation in future energy grids.

Prof Nogita’s research group leads the Hydrogen Energy node within the ARC Training Centre in Energy Technologies for Future Grids, with industries and academic collaboration including University of Wollongong and University of Tasmania.

Figures from left to right:

- *Cast Mg-Ni alloys for hydrogen storage*
- *UQ Spin-off company Hydrexia Pty Ltd*



One of the factors limiting wider uptake of H_2 in a diversified energy grid relates to difficulties in efficient storage and transport. A cost-effective H_2 storage system must possess high storage capacity, fast kinetics, long cycle life, and a good safety profile under normal use. Some of the conventional and emerging systems introduce substantial costs and/or safety issues.

Metal hydrides have been investigated for safer and more economic storage and transport of H_2 as a solid. Those based on magnesium (Mg) alloy systems show promise, but are currently held back by the high cost of energy for releasing H_2. The program will focus on identifying and implementing metal hydride systems that can be manufactured using existing technologies suitable for mass-production, rather than complex processing systems that are difficult to scale.

Direction key personnel

- **Prof Kazuhiro Nogita**
- **Dr Xin Fu Tan**

Electrochemical Energy Storage

Within the Centre for Multiscale Energy Systems (CMES), our electrochemical energy systems (EES) team conducts both fundamental and applied research, emphasising the development of advanced characterisation methods and materials design for technologies such as sodium-ion batteries, sodium metal batteries, solid oxide cells, alkaline electrolysis, and flexible batteries.

Our interdisciplinary team combines expertise from mechanical, chemical, and materials engineering, along with chemistry, to tackle pressing electrochemical energy challenges.

Our team has developed specialised operando characterisation techniques, which, paired with advanced computational modelling, provide insights into material behaviour at the molecular level guiding breakthroughs in materials design for EES.

A unique focus of CMES is understanding the mechanical failure mechanisms in battery systems that use polymer or solid-state electrolytes, addressing a key area in battery durability and performance.

We also collaborate with industry to meet large-scale energy needs, including projects for electrochemical energy solutions in remote off-grid communities and heavy-haul locomotives.

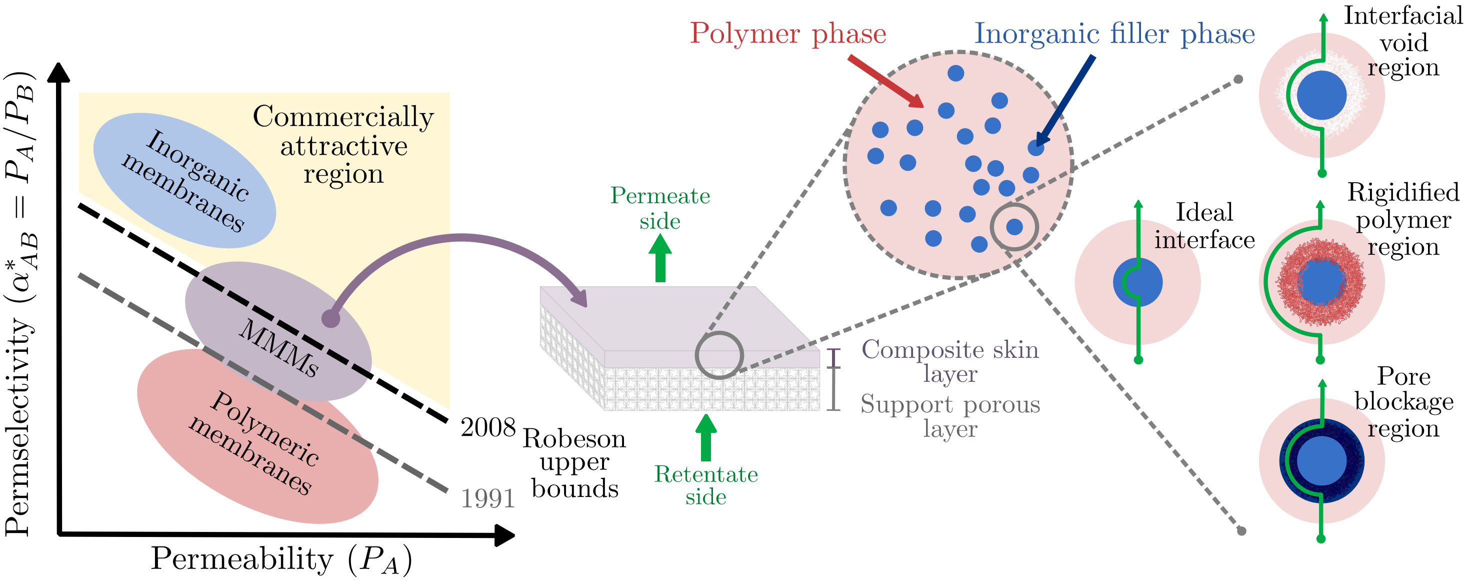
Direction key personnel

- **A/Prof Ruth Knibbe**

Transport in nanoporous materials

Nanoporous materials such as zeoloites and activated carbons have long been in industrial use as adsorbents for a variety of gas and liquid phase separations, including air separation and water purification. In recent times the urgency of arresting global warming and climate change has led to the requirement for novel energy efficient processes to capture carbon dioxide from power plant and industrial emissions and even from the air. Nanoporous materials offer much potential to address this challenge due to their established success in adsorptive and membrane-based separations. As a result there has been rapid development of materials such as metal organic and covalent organic frameworks (MOFs and COFs), zeolitic immidazolate frameworks (ZIFs), graphenes and carbon nanotubes having properties appropriate for carbon dioxide separation.

An important capability of the centre is that of the modelling and simulation of adsorption and transport in nanomaterials and membranes, with emphasis on carbon dioxide separation. In on-going research we are investigating the in silico design of a novel heterogeneous membrane, known as mixed matrix membrane (MMM), comprising an adsorbent filler such as a ZIF dispersed in a polymer matrix. Such a membrane combines the high flux capabilities of the adsorbent with the high selectivity of the polymer, and is more efficient than either ZIF or polymer-based membranes. A central challenge in MMM development is the engineering of the polymer-adsorbent interface to overcome the effects of interfacial incompatibility which can lead to selectivity reduction because of local polymer densification or the presence of nanovoids. This issue is being addressed through molecular simulation methods, which overcome the difficulties with trial and error experimentation that have been used earlier.



Considerable effort is ongoing worldwide in developing membranes of nanoscale thickness, with the aim of reducing transport resistance and thereby increasing flux and enhancing efficiency. We are examining such nanoscale membranes using theoretical models as well as molecular dynamics simulations in order to understand the complexities of interfacial resistance that arises in such membranes due to their finite size. Our work has shown that while materials such as carbon nanotubes have low selectivity at conventional membrane thicknesses of the order of tens of microns, they offer attractive prospects at nanoscale thicknesses due to the greatly different interfacial resistance for the transport of different gases. Our work aims to discover materials with potential for carbon dioxide separation at nanoscale membrane thickness and to design such membranes using computer simulation.

Direction key personnel

- **Prof Suresh Bhatia**
- **Dr Muxina Konarova**
- **Dr Gloria M. Monsalve-Bravo**

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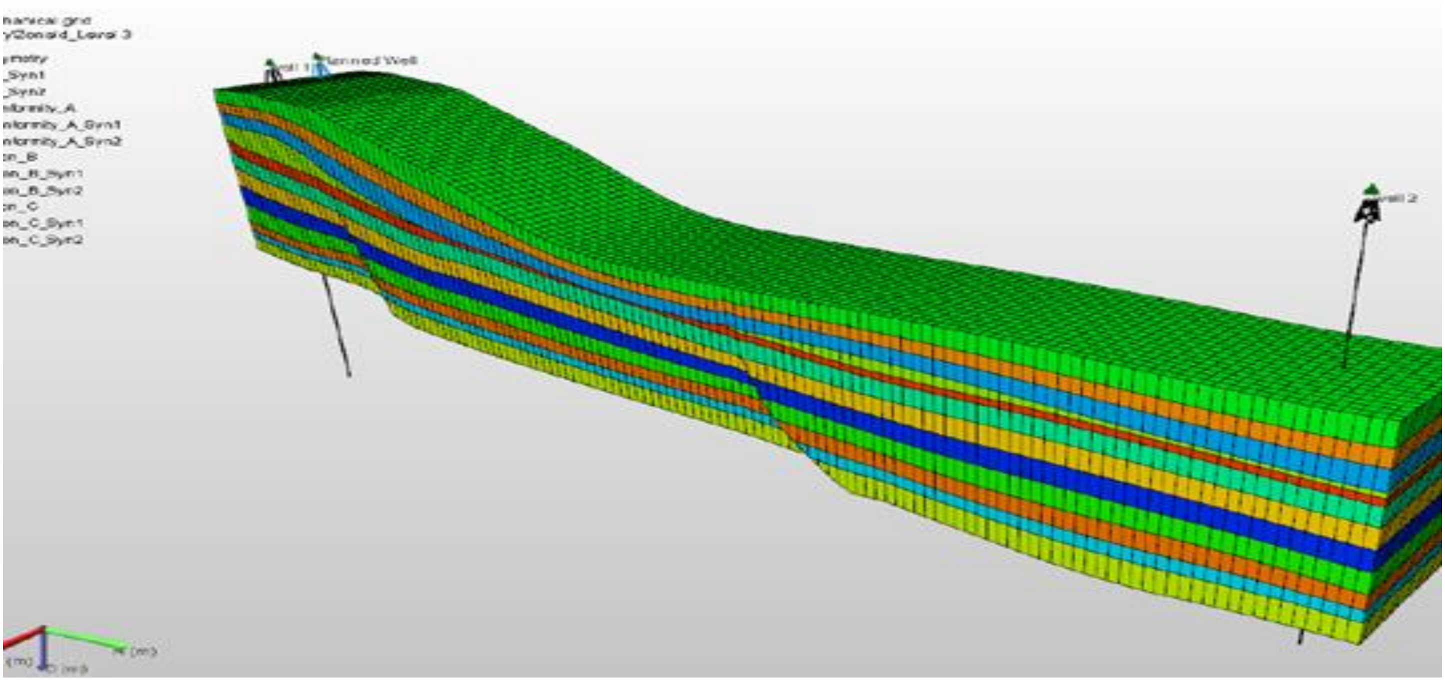


Underground Energy Storage

Within the Centre for Multiscale Energy Systems (CMES), our Environmental Geomechanics (EG) team conducts both fundamental and applied research on underground energy storage, such as Compressed Air Energy Storage (CAES) and hydrogen storage in depleted gas reservoirs or salt caverns. Our focus is on geotechnical design and environmental impact assessment to ensure each storage method is implemented in a responsible, controllable, and sustainable manner.

Our research team combines interdisciplinary expertise from wellbore drilling, geophysical logging, data-driven modelling, rock mechanics, and petroleum engineering, enabling us to effectively address the critical technical challenges of underground energy storage.

The team has developed strong experimental and numerical modelling capabilities to characterize a suite of geomaterial properties under various conditions (e.g., high pressure high temperature) and forecast fluid transport in subsurface and its long-term behaviour.

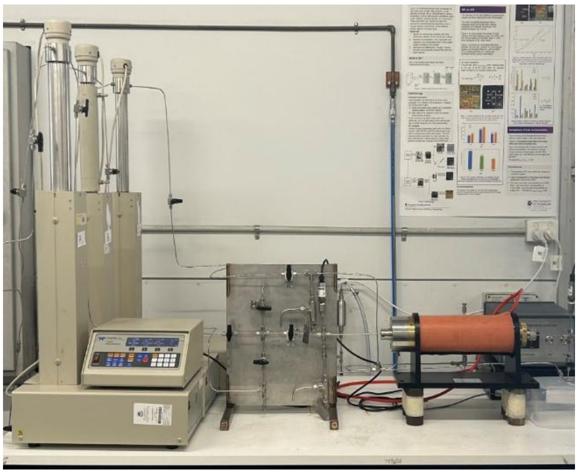
Additionally, our team maintains long-term collaborations with key gas producers in Queensland to support this strategically important research.

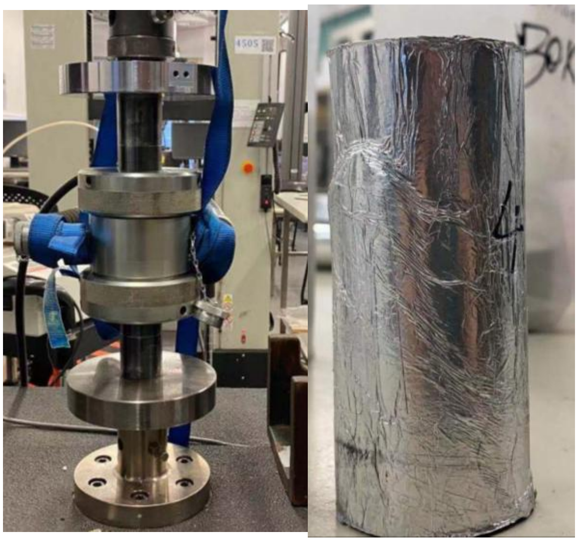
Figures from top to bottom:

- *Reservoir-scale simulation model for underground gas storage*
- *High pressure rock core flooding rig*
- *Triaxial Hoek cell for rock strength measurements*

Direction key personnel

- **A/Prof Zhongwei Chen**
- **Dr Jimmy Li**





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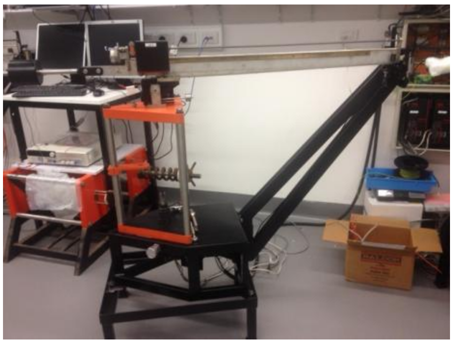
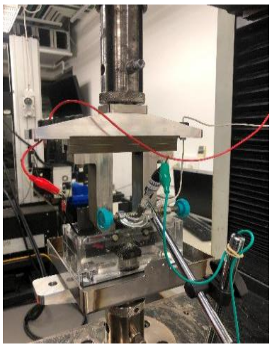
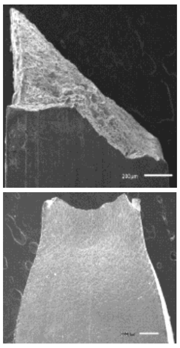
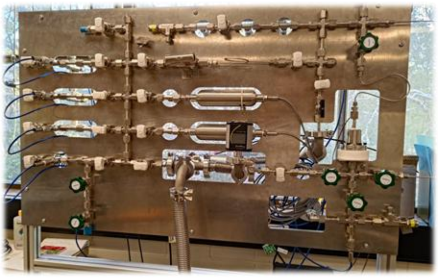
Materials Integrity Assessment

Materials are vital elements in energy systems, playing a pivotal role in establishing the infrastructure for energy generation, distribution, and consumption. One of the challenges encountered in these operations pertains to the preservation of materials integrity, specifically the prevention of undesirable materials degradation and failure during service. Material integrity challenges manifest in various forms, including the need to address stress corrosion cracking, corrosion fatigue, fatigue failures, embrittlement, and disintegration. A prime example of the necessity for materials integrity assessment is evident in the current push to embrace hydrogen energy. With the widespread adoption of the hydrogen economy in various countries, including Australia, concerns about hydrogen embrittlement have been mounting. Hydrogen embrittlement refers to the deterioration of a material's mechanical properties after exposure to even small amounts of hydrogen. This issue has been a challenge for high-strength metals, such as various steels, aluminium, and titanium alloys. Without a thorough assessment of a material's susceptibility to hydrogen embrittlement, these materials cannot be confidently utilized in hydrogen-related applications.









Figures from top to bottom:
- *Linearly Increasing Stress Test*
- *Fracture Mechanics test in hydrogen*
- *Fracture with (brittle) and without (ductile) hydrogen exposure*
- *Hydrogen gas permeation apparatus*
- *Thermal Desorption Spectroscopy*

At CMES, our researchers have proven expertise in conducting various materials integrity assessments, particularly corrosion and hydrogen embrittlement performance tests. Some of the available analytical tests include:

- Mechanical testing to assess a material's hydrogen sensitivity and stress corrosion cracking susceptibility, including the linearly increasing stress test (LIST), slow strain rate test (SSRT) and fatigue test
- Fracture mechanics analysis in hydrogen
- Hydrogen permeation tests in both electrolytic and gaseous hydrogen charging
- Hydrogen trapping analysis using thermal desorption spectroscopy (TDS)

Direction key personnel

- **Prof Andrej Atrens**
- **Dr Jeffrey Venezuela**

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