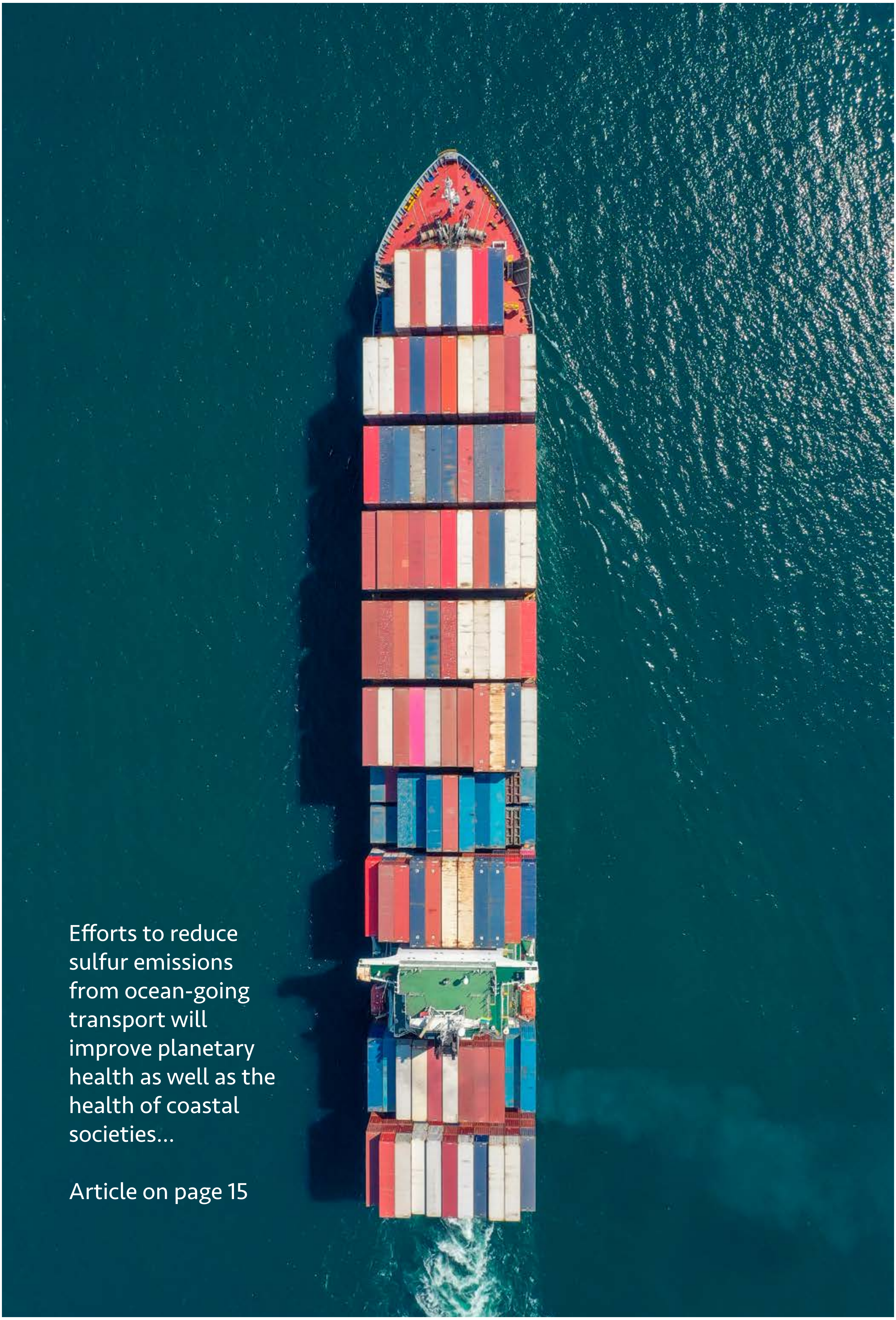
CCRC REPORT

جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology

CCRC

Winter 2023 Issue



Efforts to reduce sulfur emissions from ocean-going transport will improve planetary health as well as the health of coastal societies...

Article on page 15

A NOTE

From the Editor

The CCRC Newsletter has evolved into a new CCRC Report with an updated format and branding. This move reflects our increased use of social media to report CCRC news stories as they emerge, while in this report we document our activities, successes, and impact. The report captures many of our major engagements, research highlights and CCRC personnel news. We hope that you will take the time to flip through the report and read about our varied interests and major achievements.

CCRC has a strategic approach to work across a broad range of energy related technology readiness levels, TRLs. Combining research inquiry with technology development and scaling requires a mix of interests and experiences that CCRC is lucky to have. We cover research interests spanning the four streams of combustion research, namely, combustion fundamentals, combustion research tools, combustion applications and combustion impact and mitigation. On the fundamentals, we conduct shock tube measurements, develop detailed chemical kinetics and conduct high fidelity DNS. On the research tools, we develop advanced laser-based techniques, AI algorithms and new combustion models. While on the applications, we utilize both measurements and modeling to research plasma utilization, structure of conical flames, internal combustion engines, soot evolution, spray flames, steam calcination, hybrids of solar and combustion, fuel reforming and alterative fuels utilization. Finally, on mitigation and impact, we develop and scale technologies for cryogenic carbon capture, ultrasonic oxidative desulfurization of fuels, and electro-chemical convergence of CO2 into fuel.

Covering such fields gives our center a unique position to address major challenges related to energy conversion, now and into the future. We are also pleased that our research is making an impact both in the Saudi Arabia and the world, through our major local and international industry sponsors. Those sponsors find value in utilizing our expertise and unique facilities as well as interest in adopting our innovative technology to their operations. Our center's outward looking approach has helped in attracting and maintaining strong industry engagement over the years. We remain open to engage with interested parties for the benefits of science, industry and the environment.

I hope you enjoy this report, and are motivated to subscribe to our social media updates as well checking our website for in-depth look.

Bassam Dally
Professor of Mechanical Engineering
CCRC

Inside this Issue

CCRC REPORT:

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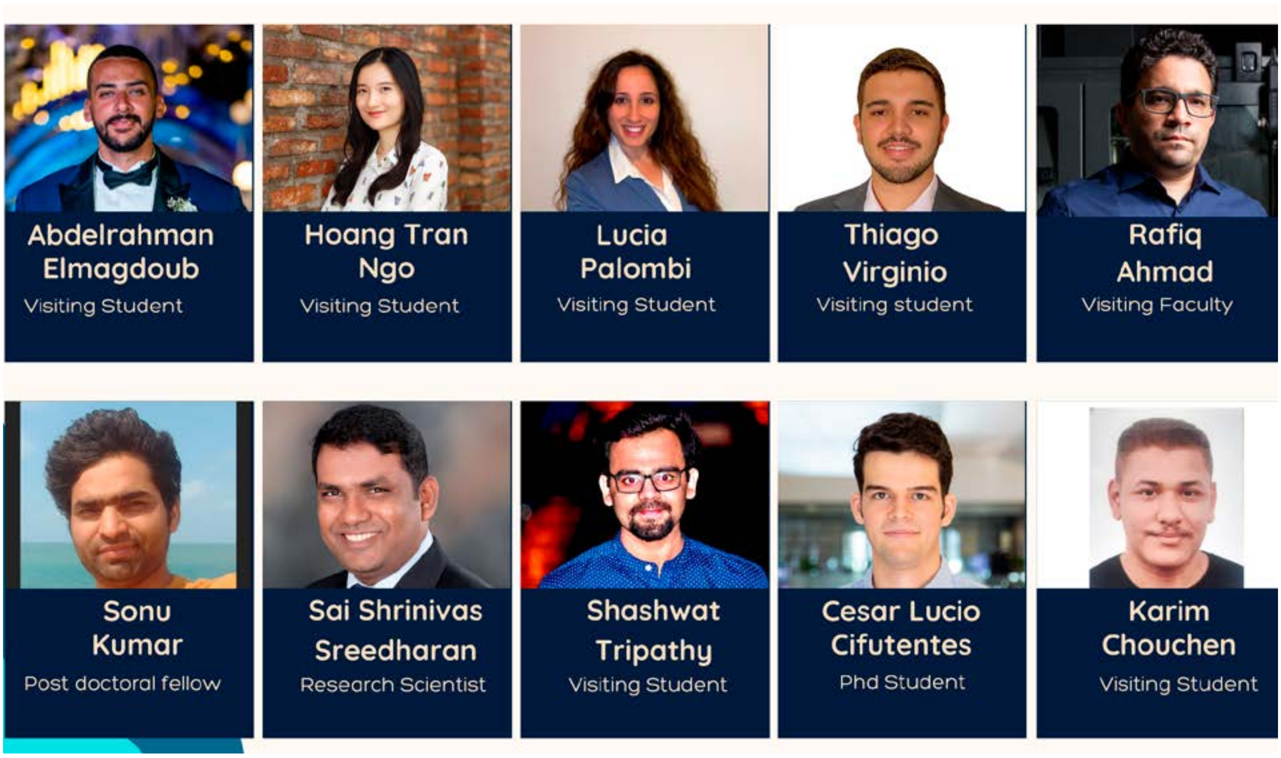
New Faces at CCRC - Welcome!



FACULTY UPDATES

Professor of Mechanical Engineering Aamir Farooq is appointed a Fellow of the Royal Society of Chemistry (FRSC)

KAUST Professor of Mechanical Engineering Aamir Farooq has recently been appointed a Fellow of the Royal Society of Chemistry (FRSC). Professor Farooq, chair of the KAUST Mechanical Engineering Program, was elected for his contributions to chemical kinetics research.

The RSC is the largest organization in Europe dedicated to advancing the chemical sciences and the professional body for chemists in the United Kingdom. As a result of his appointment, Farooq will have the opportunity to showcase his research and network with some of the world's most influential scientists.

"It is a privilege and honor to become a Fellow of the Royal Society of Chemistry. I have worked in the area of chemical kinetics and fuel chemistry for nearly 15 years, so it is a great feeling to be recognized and appreciated for my work," Farooq said of his election.

Farooq delivered a keynote presentation at one of the premier meetings of RSC where his presentation was well received by his peers. "My nomination was made by one of the top scientists in the field who attended the meeting."

"I would also like to thank my faculty colleagues, postdocs and students for their collaboration and commitment to the mission of KAUST. I would not have achieved this recognition without their contributions," he added.

Scan the QR code to read the full article

FACULTY UPDATES

KAUST Associate Professor of Mechanical Engineering Min Suk Cha has been elected as a Fellow of the Combustion Institute (CI). Cha was elected for his exceptional and innovative contributions to the fundamental understandings and advances in plasma and electrically assisted combustion.

Established in 1954, the CI is a nonprofit, international scientific and engineering society based in Pittsburgh, Pennsylvania, U.S. The Institute works to facilitate the dissemination of research in combustion science and technology worldwide. The CI views combustion research as a "field of eminent societal importance that cuts across many disciplines."

Each year, members of the CI are recognized for fellowship selection by their peers, whether in research or applications. Cha is the sixth member of the KAUST Clean Combustion Research Center (CCRC) to become a Fellow of the CI.

"It was such a rewarding moment, knowing that my 30-year-long journey through this field of study had been recognized by my peers and three Fellows who supported my nomination," he said of his election. "I am also honored to continue the CCRC's honorific record—all senior faculty have been elected as Fellows of the CI."

CCRC Professor Min Suk Cha is elected as a Fellow of the Combustion Institute

Scan the QR code to read the full article by David Murphy

FACULTY / STAFF UPDATES

Achievements / appointments late 2022-23

William Roberts

Appointed to the Combustion Institute Board of Directors

Hong Im

Appointed as Springer Professor, Mechanical Engineeing, University of California Berkeley

Bassam Dally
Appointed as president of SASCI, Technical Program co-Chair of 40th Symposium, 2024

Deanna Lacoste
Appointed as SAS-CI board member

Kevin Nall
Joined CCRC as Strategic Business Development Officer

Technology & Innovation are Key to Decarbonizing Cement

Globally, the annual production of cement exceeds 4.2 billion m^3, emitting the equivalence of 8% of the total human made CO_2. Most carbon, -60%, is emitted from the calcination of limestone ($CaCO_3$) and the rest is emitted from the burning of fossil-based fuels to produce the thermal energy needed to drive the calcination process.

A national one-day workshop organized by CCRC focused on pathways to decarbonize cement manufacturing in Saudi Arabia. The workshop is part of a center partnership fund, led by Professor Bassam Dally, to investigate strategies, technology and policies needed to develop a roadmap for cement industry in Saudi Arabia. The first of its kind in the Kingdom, the workshop was attended by 80 delegates representing all stakeholders, including government officials, all cement companies, building societies and environmental agencies.

The workshop was structured around three main themes namely, thermal efficiency &

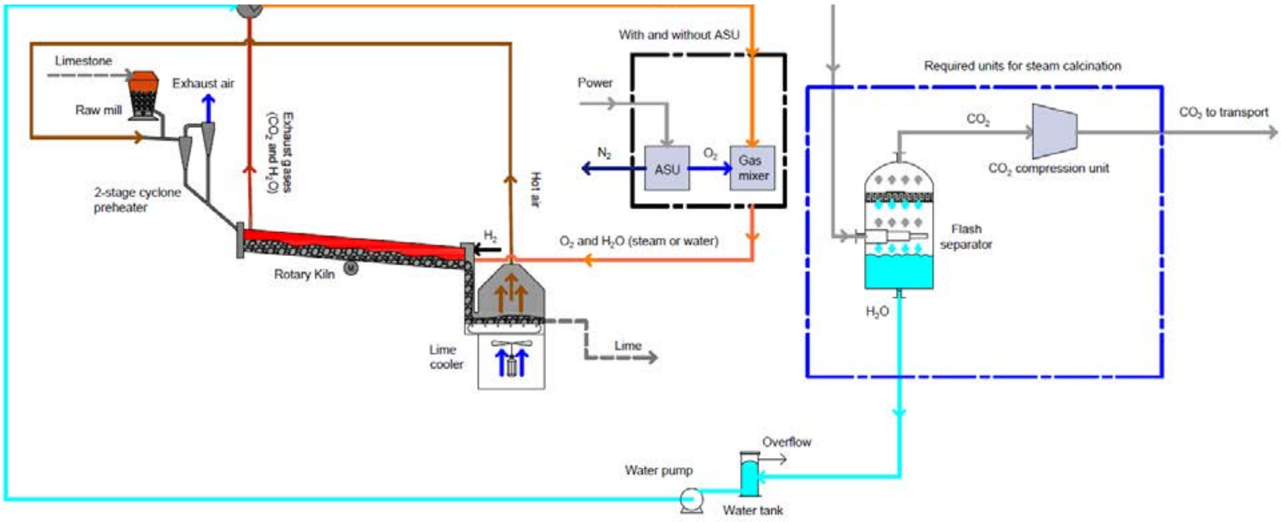


Image: Steam Calcination Patented Technology [Dally et al.]

alternative fuel, clinker substitution for carbon reduction and carbon capture usage (CCUS).

A variety of speakers covered these topics from scientific, industrial and regulatory perspectives.

Mr. Thomas Guillot, CEO of the Global Cement and Concrete Association (GCCA) gave the keynote address providing a global perspective of current and future decarbonization strategies. He also presented GCCA net-zero pathway, where improvement in energy and combustion efficiency, fuel switching and CCUS play a crucial role.

Prof Karen Scrivener of EPFL spoke of a new concrete mix that include kaolinite clay, up to 40%, which has the same strength, drying time and characteristics of a Portland cement, commonly used around the world. The proposed mix is termed Limestone Calcined Clay Cement, LC3, has been approved by many jurisdictions and included in the cement and concrete standards. By replacing limestone with clay, up to 40% reduction in CO_2 emission is expected, mostly because the process of clay calcination does not emit CO_2, beyond that used to generate the heat.

Prof Dally spoke of the new and emerging technologies to reduce carbon emission and make CO_2 capture more economical. He described the newly patented concept of steam calcination which results in an exhaust stream of pure CO_2, once water is condensed. The process was modeled using Aspen Plus and the results show that more than 90% of the CO_2 can be captured. More importantly, the majority of the condensed water, >94%, can be captured and recycled as well. This technology can result in 40% reduction in CO_2 emission, when steam is generated using renewable sources.

The workshop ended with a set of actions to further expand on the different strategies and in particular further development of the steam calcination technology to higher TRL.

Image: Musad Aldaood, Deputy Minister for Mining Development makes his opening remarks.

CCRC SPOTLIGHT

Taking Carbon Capture to the Next Level

Image: His Royal Highness Minister of Energy Prince Abdulaziz Bin Salman Al Saud officiating, MoUs signed at SGI during Cop27 between Enowa, KAUST and SEC. KAUST President Tony Chan (L), HRH Minister of Energy (M); and SEC Executive Vice President, Distribution and Customer Service, Ibrahim M. Al-Khenizan (R).

In what will be one of the largest demonstrations of cryogenic carbon capture technology today, a pilot project between King Abdullah University of Science and Technology (KAUST), ENOWA, (NEOM's Energy & Water company), and the Saudi Electricity Company (SEC) is expected to capture 30 tonnes of carbon dioxide per day from SEC's Green Duba Integrated Solar Combined Cycle (ISCC) power plant at NEOM.

In an official ceremony at the Saudi Green Initiative Forum 2022 during COP27 in Sharm El Sheikh, Egypt, with His Royal Highness Minister of Energy Prince Abdulaziz Bin Salman Al Saud officiating, the signing of two significant documents puts years of dedicated research and development into practice, and underscores the commitment of the Kingdom of Saudi Arabia to move from "ambition to action" with its climate action plans.

Cryogenic carbon capture technology is a highly energy efficient and low-cost process with the potential to radically reduce carbon emissions, and, therefore, the carbon footprint of the Kingdom. The carbon captured at the pilot plant is then ready to transport as pure liquid CO_2 at room temperature, suitable for food and beverage applications, and with the majority used to produce e-fuels designed to replace fossil fuels for internal combustion engines.

Saudi Electricity Company will build and operate the pilot plant. All three partners are committed to the global momentum to increase the use of efficient and affordable carbon capture technology.

Soon after COP27 in December 2022 CCRC celebrated the CCC project with a ribbon cutting and an unveiling of the new CCC technology rig that will also be deployed for the first time at

Image L-R: Tony Chan - KAUST President , William Roberts - CCRC Director, Khaled Al-Ghamdi - VP of Technical Services - SEC, and His Excellency Osama bin Abdulaziz Al-Zamil cut the ribbon on the CCC rig.

the power plant in Rabigh to demonstrate the transportablility of the technology.

KAUST Professor William Roberts, director of the CCRC whose expertise in cryogenic carbon capture technologies leads the project, said: "Together we can play a pivotal role in achieving the "net-zero" emissions goal of the sustainable energy future. The signing is a recognition of the years of world-class research and extensive collaboration by so many people at KAUST, Sustainable Energy Solutions (SES/Chart, our technology partner), SEC, NEOM, the Ministry of Energy and NIDLP."

Image: CCRC unveils the cryogenic carbon capture rig in December 2022 with high-level guests from the Kingdom

Scan the QR code to see the video

CCRC SPOTLIGHT

Hydrogen-Based Mobility & Power Conference

October of 2022 had delegates from academia, government laboratories, and industry attend an in-person conference on 'Hydrogen-Based Mobility and Power' at KAUST, hosted and organized by the CCRC.

The conference was organized around three areas:

1. Use of Hydrogen for Mobility and Power Generation
2. Production and Availability of Hydrogen with Zero Carbon Impact
3. Issues Surrounding the Utilization of Hydrogen from an Infrastructure Standpoint

Two highlights bookended the conference. Firstly, the keynote given by Prof. Helmut Eichlseder from the University of Graz. Eichlseder spent many years researching hydrogen as a fuel for spark-ignition engines and previously worked closely with BMW in this area. He provided a comprehensive overview of what was done in the past, the challenges being faced now, and the main research topics in the area of transportation using hydrogen in the future.

The other highlight was the final presentation from Reliance Industries. They introduced their new repowering program for existing diesel trucks in India, primarily to allow hydrogen to be used to the benefit of air quality. This was the world's first reveal of this major initiative to improve the quality of life of Indians living in the country's heavily polluted cities, and as such, a major outcome.

There were also presentations from Bosch on their fuel injection equipment, power generation from UC Irvine and Korea Institute of Energy Technology, as well as BP presenting on the outlook for hydrogen in future mobility scenarios.

Scan the QR code to watch the presentations on Youtube

22 e-poster presentations

27 speakers over 3 days

459 in-person registered

CCRC SPOTLIGHT

CCRC Advisory Board Meeting November 2022

Advisory Board members and members of CCRC at the meeting held at KAUST
L - R: Andrew Maloney, Saumitra Saxena, Professor Xu Lu, Professor Mani Sarathy, Mohammed Juaied, Professor Aamir Farooq, Ahmed Al-Saggaf - Director of Innovation at SGS, Malik Aqel - Manager of Strategy and Business at Maaden, Professor Bassam Dally, Catherine Owen, Kevin Nall, Gerard de Nazelle - Head R+D Saudi Aramco, Turki Albabtain - Advisor Ministry of Industry and Mineral Resources

The CCRC Industry Advisory Board met at KAUST and virtually in November 2022. Eighteen industry and KAUST faculty/staff attended the meeting to report on and celebrate the many achievements of the Center in the past year. Center Director Bill Roberts provided an impressive summary of Center activities in the areas of faculty achievement, graduate success as well as Center leadership nationally and internationally.

Professor Aamir Farooq provided an update on the Fluids, Lubricants, Efficient Engines, Technology (FLEET) Consortium which consists of six industry partners; Toyota, Saptco, Hyundai, Bahri, Pacific Green and Aramco. Two new partners joining for the upcoming year are Ferrari and Luberef. Additional presentations were provided by Professor Mani Sarathy on Sustainable Aviation Fuels Formulated by Artificial Intelligence and Professor Bassam Dally presented on CCRC's expansion into the mineral industry in KSA.

Board Chairman, Dr. Gerard de Nazelle, recognized that CCRC is one of the top combustion research centers in the world. Additionally, he led a spirited discussion of the criticality of academia engaging in deployable or applied research that can make a commercial impact in the Kingdom and the world. He believes strongly that CCRC excels in this area and encourages both CCRC and the Advisory Board to continue down this path.

Air Products volunteered to host the Spring 2023 Board meeting at their Allentown, Pennsylvania corporate headquarters.

CCRC SPOTLIGHT

Hydrogen Seminar Series

A fortnightly series of 7 hybrid seminars (in-CCRC CCRC held a fortnightly series of fall seminars in the second half of 2022 titled the Hydrogen Seminar Series (HSS). The goal was to bring together leading experts in hydrogen from government, national labs, academia, and industry to provide critical insights into the technology, economics, policy, and market including business drivers and barriers for hydrogen, both in the short term and in the long term.

During the seminars, speakers examined hydrogen production, transportation, storage, distribution, safety, use, and commercial opportunities, as well as the policy levers that are necessary to accelerate the deployment of hydrogen.

Scan the QR code to watch the presentations or view slides

7 seminars

21 speakers

+3000 registered

CCRC SPOTLIGHT

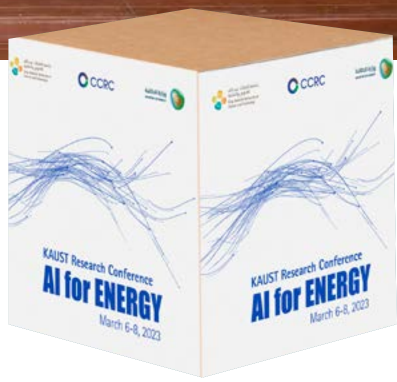
Ammonia workshop - September 2022

Between KAUST and Tohoku University (IFS) a core-to-core workshop took place at KAUST in September of 2022 over a couple of days. This hybrid workshop consisted of 8 session chairs, 30 speakers and 12 e-poster presenters as well as lab tours around the CCRC facilities.

Participants came from institutions far and wide that included Tohoku University, Hokkaido University, Hiroshima University, Kyushu University, AIST, University of Orleans, CNRS-Orleans and KAUST. The workshop was open to all CCRC members.

CCRC SPOTLIGHT

AI for Energy Conference - March 2023



How can AI assist in the design of new fuels, and integrate hydrogen and renewables into the energy landscape? This question and others spanning the advances of AI for applications in the storage and conversion of energy were unpacked at the recent KAUST Research Conference on AI for Energy hosted by CCRC in March this year.

Bringing together worldwide experts from academia, industry, and government to discuss applications of Artificial Intelligence in the broad field of energy, the conference was formally supported by the Ministry of Energy (MoE). They contributed by selecting 8 speakers from various Saudi institutions including the Ministry of Energy (MoE), Saudi Aramco, SDAIA, SABIC, CNTXT, and SEC and also advertised the conference through their channels.

Energy is one of KAUST's pillars and Artificial Intelligence has become an important theme at KAUST, as evidenced by the inauguration of the KAUST AI Initiative and by the creation of a fifth KAUST pillar on the Digital domain. These two pillars were brought together through the conference's three topical areas:

(1) AI for fuel and engine design,
(2) AI for hydrogen and renewables, and
(3) AI for sensing and diagnostics in energy-related applications.

Speakers and delegates from leading universities in USA, Europe and Asia attended the three day conference at KAUST, where they exchanged views, networked and planned future collaboration. A new collaboration on high-pressure ammonia combustion between CCRC and Staford personnel has started on the back of the AI for Energy conference.

Presentations from the AI conference will be available on Youtube soon

Waves Of Change Reduce Emissions From Shipping

Image: Mohammad Al Tayyar and Professor William Roberts

A fruitful research consortium that aims to develop cleaner marine fuels was sparked by the need to comply with new regulations for sulfur emissions introduced in 2020 by the International Maritime Organization.

To help meet these new regulations, KAUST is partnering with the Oil Sustainability Program and Saudi Aramco's base oil company Luberef. Together, they are undertaking the first demonstration step of fuel desulfurization at the refinery scale.

Sulphur dioxide (SOx) is one of the greenhouse gases implicated in climate change. Thus, lowering these emissions to below the regulated 0.50 percent will improve air quality and reduce acidification of coastal waters — a good outcome for coastal communities as well as the planet.

"Options to reduce SOx emissions are currently limited and impractical for an industry like shipping that is a low-margin business," explains William Roberts, director of the Clean Combustion Research Center at KAUST. For example, retrofitting for a low-emission fuel or installing exhaust cleaning systems would require costly vessel upgrades and take decades.
"The most cost and time effective alternative is to tinker with the heavy fuel to remove the sulfur," says Roberts. KAUST is researching such an option through the spinout company uODS, led by Roberts, in collaboration with the Oil Sustainability Program and Luberef.

"This is where real impact happens," suggests Mohammad Al Tayyar, program director of the Oil Sustainability, speaking about the importance of this project to address a global challenge. "We need to scale up technologies from the lab all the way to commercial applications that can be deployed globally."

"This is connected to the Kingdom's Vision 2030, as we are utilizing hydrocarbons in the most environmentally and economically sustainable manner," says Al Tayyar...

Scan the QR code to read the full article and watch the video

RESEARCH UPDATES

AI Screens To Make Transport Fuels Green

An inverse mixture-design approach based on machine learning can teach computers to create mixtures from a set of target properties. Developed by KAUST, this could help find high-performance transport fuels that burn efficiently while releasing little carbon dioxide (CO_2) into the atmosphere.

Greenhouse gas emissions are major contributors to rising global temperatures. A large proportion of CO_2 emissions comes from the combustion of hydrocarbon fuels, such as gasoline, that power most automotive engines. A promising solution to these environmental issues is to engineer transport fuels that offer enhanced efficiency and lower carbon emissions.

There are several methods developed for fuel screening, but they are usually validated only on smaller blends, or require additional preprocessing, which makes these configurations unsuitable for inverse fuel design. "The key bottleneck is screening complex mixtures containing hundreds of components to predict synergistic and antagonistic effects of species on the resultant mixture properties," says first author Nursulu Kuzhagaliyeva, a Ph.D. student in Mani Sarathy's research group.

Kuzhagaliyeva, Sarathy and coworkers constructed a deep learning model — comprising multiple smaller networks dedicated to specific tasks — to screen fuels efficiently. "This problem was a good fit for deep learning that allows capturing nonlinear interactions between species," Kuzhagaliyeva says. In the inverse-design approach, the researchers first defined combustion-related properties, such as fuel ignition quality and sooting propensity, and then determined potential fuels according to these properties.

Publicly available experimental data are scarce. Therefore, the researchers built an extensive database using experimental measurements from the literature to train the model. The database consisted of different types of pure compounds, surrogate fuel blends and complex mixtures, such as gasoline.
There was no model adaptable to inverse fuel design, so the researchers had to embed vector representations in the model, Kuzhagaliyeva says. Inspired by text processing techniques that relate words to phrases using hidden vectors, they introduced a mixing operator that directly connects hidden representations of pure compounds and mixtures through linear combinations. They also added search algorithms to detect fuel mixtures that match the predefined properties within a chemical space.

The model accurately predicted the fuel ignition quality and sooting propensity of various molecules and mixtures. It also identified several fuel blends fitting the predefined criteria.

The team is now enhancing model accuracy by extending the property database to other criteria, such as volatility, viscosity and pollutant formation. The tool is being advanced to formulate gasoline e-fuels and synthetic aviation fuels. "We are also developing a cloud-based platform to enable others to use the tool," Kuzhagaliyeva says.

Article by: Nursulu Kuzhagaliyeva, PhD student.

References:
Kuzhagaliyeva, N., Horváth, S., Williams, J., Nicolle, A. & Sarathy, S.M. Artificial intelligence-driven design of fuel mixtures. Communications Chemistry 5, 111 (2022).
| article

"C7" Sub Mechanism Completes the Puzzle of Nierarchical Aromatic Chemistry

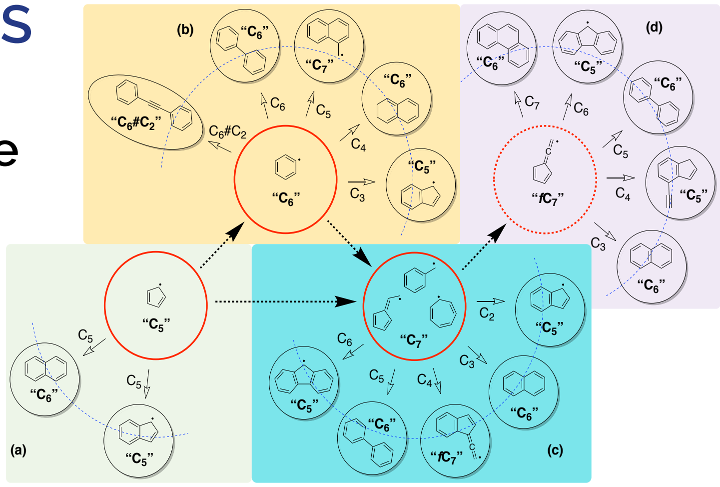


Image: Hierarchical reaction network of monocyclic aromatic hydrocarbons. Molecules in red circles are the basic aromatic classes of "C5", "C6", "C7", and "fC7"; dotted arrows indicate internal conversion; hollow arrows indicate cross-level pathways.

The emission of soot nanoparticles has been a major concern of conventional combustors for decades due to the hazardous impacts of soot on climate, environment, and human health. Numerical simulations using kinetic models can be used to predict soot concentration and tailor the combustion process in new combustor designs. A better understanding of the formation chemistry of soot nanoparticle is, therefore, beneficial to the reduction of the emission of this pollutant. Polycyclic aromatic hydrocarbons (PAHs), serving as soot precursors, have been investigated extensively to illustrate their chemistry of formation and aggregation.

PAHs are formed via complicated chemical processes from fuel molecules, including the initial gas-phase reactions, the first aromatic ring formation, and the aromatic growth. Benzene / phenyl ("C6") and cyclopentadienyl ("C5") are considered as the critical first aromatic rings formed. In our work, we upgraded the commonly undervalued sub-mechanism of "C7" aromatics (vinyl-cyclopentadienyl, tropyl, fulvenallene, and fulvenallenyl) and combined it with "C5" and "C6" chemistry to reveal the basis of aromatic chemistry.

The entire aromatic chemistry consists of three characteristic ring styles, cyclopentadienyl, phenyl, and tropyl, and is divided into several hierarchical reaction networks based on the number of aromatic rings. Taking monocyclic aromatic hydrocarbons (MAHs) as an example, their basic aromatic classes are "C5", "C6", "C7", and "fC7", shown in Fig. 1. The reactions between the basic aromatic classes and other aromatic species in the same hierarchical level are designated as internal conversion; reactions from one hierarchical level to other levels are called cross-level pathways. Internal conversion does not directly contribute to PAH growth but serves to keep thermodynamic balance of the carbon flux among the same aromatic level. On the contrary, cross-level pathways provide almost all efficient PAH growth starting from the basic aromatic classes. These reactions fuse at least one new aromatic ring, which regain basic aromatic classes of the higher levels. Furthermore, the hierarchical reaction network has the feature of self-imitation. For bicyclic aromatic hydrocarbons (BAHs), "C5" is indenyl, "C6" is naphthyl, "C7" are $C_{11}H_9$ aromatic species, and "fC7" is benzyl-fulvenallenyl. The cross-level pathways of BAHs are very similar to those of MAHs, with few unique features due to the presence of zigzag, armchair, cove, and fjord peripheries with increasing aromatic rings.

Model development has commonly been guided by the strategy of PAH formation pathways. Therefore, every aromatic radical has a chance to be the precursor of PAH and soot, and every reaction between two intermediates has a chance to be the formation pathway of PAH and soot. Due to the infinite number of aromatic species, the identification of PAH growth pathways is an endless and time-consuming task. Such a model development strategy is generally applicable for all chemically reacting systems, it, however, ignores the nature of aromatic hydrocarbons at some level. Our model is developed using a two-dimensional strategy, considering the importance of basic aromatic classes and cross-level pathways. All aromatic hydrocarbons are grouped with aromatic rings, and organized in different hierarchical reaction networks. These hierarchical reaction networks of different aromatic levels self-imitate each other, and connect to each other by cross-level pathways originated from the basic aromatic classes. Therefore, this model is named as the Hierarchical Aromatic-Soot (HAS) model. The current work is limited to PAH chemistry, but this strategy can be expanded to close the gap between PAH and soot nanoparticles.

Article by Hangfen Jin, Research Scientist

References:

1. H. Jin, A. Farooq, C7 reaction mechanism and its self-imitation in the kinetic modeling of PAH formation, Combust. Flame (2023), in press.

Laser Imaging Helps Clean Fuels Live Up to Their Reputation

Image: Instantaneous laser image of a flame produced by combusting ammonia. The flame is disturbed and wrinkled due to turbulence. © 2022 KAUST.

Using ammonia as a hydrogen-rich energy source requires technology that can spot pollutants in flames.

A technique that enables KAUST researchers to identify two kinds of pollutants with a single laser beam could make it easier to generate heat and power from ammonia, a carbon-free hydrogen carrier.

An important component of the nitrogen fertilizer industry, liquid ammonia carries more hydrogen in a set volume than liquid hydrogen itself. Analysts predict that, with established production, transportation and storage bases, ammonia could help bring hydrogen-powered engines into the power and mobility markets.

But realizing this goal requires researchers to face a burning issue: the combustion process that generates heat from ammonia can also produce nitrogen oxide pollutants that are known environmental toxins. "If you're not careful, your ammonia flame can be just as bad for global warming as oil or natural gas, even though there are no CO2 emissions," says KAUST's Thibault Guiberti.

Guiberti and his colleagues are working to solve this problem with a technique that flattens a typical laser beam into a two-dimensional plane. By directing this sheet-like beam into a burning flame, the researchers can stimulate specific compounds in thin sections of the flame to emit fluorescent light. High-sensitivity cameras capture changes in fluorescent light intensity for different regions and heights of the flame.

"We record the fluorescent light for only a few tens of nanoseconds, so we get an instantaneous picture of where the gas is in space," says Guiberti. "You can image species that have very low concentrations, sometimes down to part per billion levels."

Most planar laser-induced fluorescence (PLIF) systems contain a single laser, meaning only one target at a time can be imaged. The KAUST team recently discovered a way to overcome this limitation using optical techniques that split a single laser into two beams with different, but predictable, energy variations. Using simulators and experimental data, the researchers studied two components of ammonia flames — the nitric oxide (NO) and imidogen (NH) radicals — and identified a setup that could energize both particles to fluoresce simultaneously.

Images taken with the new PLIF technology provided remarkable details about the inner structure of ammonia flames. "You can see the corrugated and wrinkled NH signal; that's where the flame is," explains Guiberti. "The NO is produced within the flame, and we can see how turbulence affects the flow of this pollutant."

Guiberti anticipates that this effect, which they term a "spectral coincidence," could be extended to excite even more species in ammonia flames and other low-carbon fuels.

Article by: Thibault Guiberti, Assistant Research Professor

References:

Wang, G., Shi, H., Roberts, W. L. & Guiberti, T.F. Simultaneous imaging of NO and NH in an ammonia-hydrogen-nitrogen flame using a single dye laser. Combustion and Flame 245, 112355 (2022).| article

RESEARCH UPDATES
Plasma, Humanity's New Fire?

Plasma-based processes are a potential key technology to enable the electrification of energy-intensive sectors that are difficult to decarbonize. Its potential ranges from transforming electrical energy into chemical energy by synthesizing e-fuels and e-chemicals, to processing metal ores and catalytic materials.

CCRC researchers from the Plasma Assisted Combustion Lab, led by Professor Min Suk Cha, established a combined experimental and modelling platform to study these promising temperature-dependent plasma-assisted processes.

"Plasma discharges provide us with the unique opportunity to control the chemistry in two ways, through electron-induced and thermally-induced reactions," says Cha. "To design and improve these plasma processes, we need to understand what is happening on a chemical level."

Image: Temperature-controlled dielectric barrier discharge (DBD) reactor

To date, however, research focused mainly on either highly diluted, room temperature, or low-pressure conditions. Therefore, the team from CCRC developed a numerical tool to study the temperature dependence of the plasma chemistry, called KAUSTkin. KAUSTkin is a zero-dimensional plasma-chemical kinetic model that couples ZDPlasKin and Chemkin. ZDPlasKin handles the electron-induced reactions and Chemkin the thermally-driven reactions.

Naturally, the strength of any numerical tool depends on its ability to represent reality. Thus, Professor Cha's team also designed a temperature-controlled dielectric barrier discharge reactor that allows them to determine the key plasma discharge properties, such as breakdown voltage and reduced electric field, while maintaining full control over the pressure, temperature and discharge power.

"With this combined experimental and modelling platform, we were all set to unravel the plasma chemysteries for plasma systems ranging any where from 300 to 1200 K," says Dr. Ramses Snoeckx (Research Scientist in Cha's team).

To put their approach to the test, the team chose H2 and O2 as foundational building blocks. They developed a comprehensive temperature-dependent plasma-chemical kinetic reaction mechanism for H2/O2 mixtures by investigating the oxidation of H2 for different equivalence ratios. Groundbreaking was the observation of Negative Temperature Coefficient (NTC)-like behavior. This never-before-observed phenomenon was explained by the low-temperature initiation of the oxidation process through electron-induced reactions, a pathway that is not accessible to the conventional thermal oxidation process.

After the successful validation of the H2/O2 building block, the team, including PhD Students, Seunghwan Bang and Aswath Mohanan, are now working on both carbon (CO2, CH4, higher hydrocarbons and alcohols) and nitrogen (N2, NOx and NH3) containing systems.

"Considering the analogies with combustion and its large potential, plasma could be considered as a future, more adaptive alternative to fire," Cha says.

Article by Andrea B. M. Hulsbosch

RESEARCH UPDATES

Simple Electrochemical Reactor Helps LITHIUM EXTRACTION

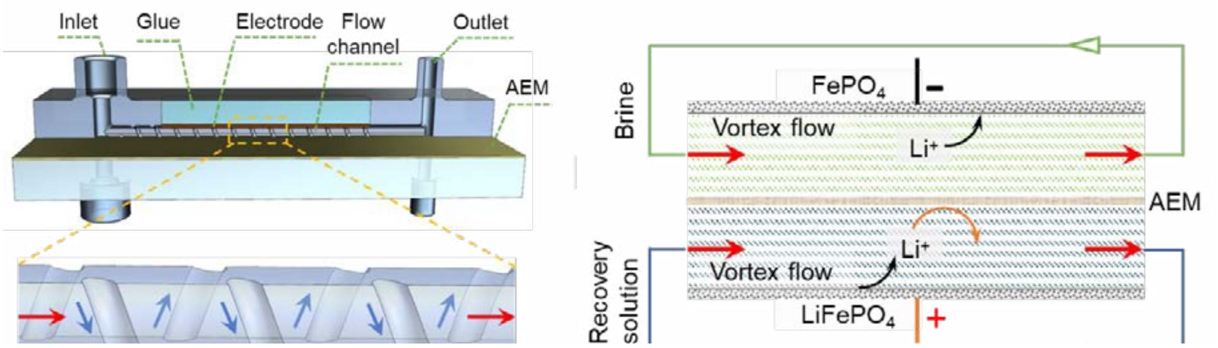


Image: Design of the SMER with a zoomed-in view of the spiral microstructures on the flow channel walls and schematic of the Li extraction process in SMER with forced vortex.

A novel spiral-microstructured electrochemical reactor has been designed by KAUST researchers to accomplish solar-driven ultrafast and economical Li extraction under harsh brine conditions, providing a sustainable and feasible roadmap to meeting the global Li demand.

Lithium (Li) is considered the "white petroleum" of current energy sector, as it is the primary component of Li-ion batteries used for electric vehicles, portable electronics, and renewable energy storage.

To satisfy the ever-growing demand for battery-grade Li2CO3, electrochemical extraction of Li from low-grade salt lake brine, powered by off-grid renewables, has been proposed as a possible solution. Yet, this technology is beset by the low extraction rate and high production cost, due to the lack of research into reactor engineering and system scalability.

Despite some notable progress in designing Li-selective adsorption/desorption materials, such as FePO4/LiFePO4 and LiMnO2/λMnO2, electrochemical Li extraction from low-grade salt lake brine has not yet been commercially viable. It was revealed that the limiting step is no longer the intrinsic Li adsorption/desorption capacity of electrode materials; instead, it is the sluggish Li-ion transport in the supporting aqueous electrolytes that leads to low Li extraction rates below 3.9 milligram of Li per gram of active materials per hour (mg g-1 h-1), far from being industrially mature.
Now, Group Xu Lu from the KAUST Clean Combustion Research Center, in collaboration with Group Stefaan De Wolf from KAUST Solar Center and Group Zhiping Lai from the KAUST Advanced Membranes and Porous Materials Center, have demonstrated an ultrafast and economical Li extraction from low-grade salt lake brine using a solar-driven and scalable spiral-microstructured electrochemical reactor (SMER).
Compared to state-of-art technologies, the SMER exhibited over 5.6-fold increase in the Li extraction rate of 21.96 mg g-1 h-1, while preserving high product purity. The SMER could be easily up-scaled for commercial production of battery-grade Li2CO3 driven by solar cells. A module consisting of four SMERs connected in series and parallel, powered by an off-grid perovskite/silicon tandem solar cell, has been shown to stably output battery-grade Li2CO3 with a low carbon footprint.

The researchers used fluid simulation and electrochemical analysis to clarify that the designed spiral microstructures on the flow channel walls in the SMER created forced vortex to enhance the Li+ mass transfer, which favored the Li adsorption/desorption processes and increased the ionic conductivity of electrolytes, and therefore substantially accelerated the Li extraction rate.

They also found that the SMER assembly using integrate technology could produce Li2CO3 with a plant-gate production cost of $28.55 kg-1, as indicated by the TEA. The up-scaled SMER assembly, with a notable gross profit rate of 149% and a short payback period of only one year, provides a sustainable and feasible roadmap to meeting the global Li demand from low-grade salt lakes and can be readily transferred to most Li reserves/resources that are more minable.

Published on: X. Zhang, Z. Li, J. Liu, F. Xu, L. Zheng, S. Wolf, Z. Lai, X. Lu. Solar-driven ultrafast lithium extraction from low-grade brine using microfluidics-mediated vortex in scalable electrochemical reactors. Chemical Engineering Journal 454, 140074 (2023). article

STUDENT LIFE

CCRC Winter School 2022

What does it take to become a combustion researcher? Eight students were able to find out during a 3-week immersion in the CCRC's cutting-edge combustion winter school for bachelor and master students.

Sponsored by the VSRP Office the Wnter School provides increased visibility for KAUST and the CCRC among potential PhD applicants from targeted regions. To date there have been four editions of the winter school hosting a total of 47 students: 2018 (15), 2019 (15) , 2020 (9), 2022 (8).

Notably, one of the first students to attend the 2018 Winter School defended his PhD dissertation in November 2022.

STUDENT LIFE

Student Advisory Committee Transforms

Image L-R: Dr Bin Wu (Post doc) Michael Oyinloye (PhD student, Chiara Canciani (PhD student) Zeniab Al Hadi (PhD student), Dr. Inna Gorbatenko (Post doc), Jordan Figueiredo (PhD student, Ammar Alkhalifa (PhD student)

The CCRC Student Advisory Committee has undergone a significant transformation. To better serve not only the student body, but also the post-doctorate fellows and research scientists, and improve the committee's impact, they decided to change the structure and also to rebrand the committee to reflect the changes. Now named the Center Engagement Committee (CEC), they believe this better reflects their mission and vision. CEC also welcomed post-doctoral fellows Dr. Inna Gorbatenko and Dr. Bin Wu as new members - the first time postdocs have been represented in this way.

CCRC Football Team Wins a Bronze Medal

The CCRC finished 3rd place after beating Security 9-1 in the 3rd place play off in an inter-departmental football tournament. The team made up of students, faculty and staff came away with a bronze medal. A first for the team!

FEATURED ALUMNI

Erica Quadarella

PhD 2022
Program: Mechanical Engineering
PI: Prof. Hong Im
Current Position: Postdoctoral Researcher - KAUST

The beginning at KAUST was challenging, as it was my first time living abroad in a different country. I gave myself time to understand if this was the right choice, and thanks to KAUST, the CCRC, and the people, I've realized how lucky I was to get this opportunity.

The stories of people I have met here represent a precious wealth of knowledge. The chances for personal and professional growth offered by this place allowed me to complete my PhD more aware of my capabilities and what I desire for my future.

Over time I became independent and critically active in research, learning to be more thoughtful and rational when tackling a challenge, and developing new ideas for upcoming projects.

Paolo Guida

PhD 2021
Program: Mechanical Engineering
PI: Prof. William L. Roberts
Current Position: Research Scientist - KAUST

My experience as a PhD student at KAUST was extremely intense. I had the opportunity to meet numerous fantastic people working in academia and industry and participate in many different projects.

One of the things I appreciated most was the continuous exposure to real-world problems and responsibilities. The ideas generated during the past five years at KAUST eventually grow into startups, and I decided to stay here to help realize one. The KAUST environment favors the creation of new technologies and finances businesses thanks to programs like Taqadam. Also, KAUST is packed with experts in every possible field, which significantly helps. In the future I will be moving forward with the realization of various projects.

Image: Paolo and Erica met while doing their Master's at Politecnico di Milano. In January 2023 they were married in Rome. In CCRC family style both their PI's and other CCRC members travelled to Italy to celebrate with them.

Erica Quadarella continues...

The truth is that, while I was a little scared by research at the beginning, it now boosts me every day to do better and makes me feel part of scientific progress. The way KAUST puts students in continuous contact with other universities, research groups, and industries allowed me to better understand where this progress is directed and be more aware of the fields where I want to concentrate my efforts in the future.

I am thrilled to continue my journey here as a Postdoc, and I can't wait to see myself in this new role. There are new projects that will allow me to see my research work directly applied to industrial processes and to try my hand at developing software for commercial use.

UPCOMING EVENT

CCRC will host a Combustion Institute-Summer School (CI-SS) on Carbon Free Combustion from May 21 – 25, 2023.

For more details and to register scan the QR code

The Summer School will provide a good overview of :

- **Combustion fundamentals**
- **Optical diagnostics**
- **Fuel Chemistry**
- **Novel Applications**