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

KAUST SUMMER 2018

CCRC Clean Combustion Research Center

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The winter school class at a desert camp

Clean Combustion Winter School

CCRC hosted 15 undergraduate students from all over the world for the first Clean Combustion Winter School. During this three-week event, students were exposed to challenges and opportunities in combustion research, both in theory and in practical applications.

Last January, the CCRC hosted 15 undergraduate students from all over the world for the first Clean Combustion Winter School. During this three-week event, students were exposed to challenges and opportunities in combustion research, both in theory and in practical applications. Each week was dedicated to a specific research topic in engines, flames or fuels.

Morning lectures addressed research topics from CCRC members, covering aspects of combustion from fundamental flame theories and detailed kinetic models to advanced engine experiments and 3D simulations. Projects were assigned and students were divided into groups of three; afternoons were devoted to hands-on research. Experiments and simulations were performed in the state-of-the-art facilities at KAUST.

At the end of each week, student groups presented their project to a committee of CCRC members. Giuseppe Indelicato (Italy), Paula Daniela Pico Viviescas (Colombia), and Yulanderson Salguero Rodriguez (Colombia) each received an iPad for their winning project: "Rayleigh scattering for temperature measurements in turbulent flames".

"The competition was friendly, but the students took the lab projects very seriously. Giuseppe, Paula, and Yulanderson were new to laser diagnostics; their backgrounds are aerospace engineering and chemical engineering. But they showed impressive results in this three-day project, confirming that an interdisciplinary approach is good strategy for tackling complex problems", said Prof. Deanna Lacoste, who co-organized the event with Prof. Gaetano Magnotti.

Giuseppe Indelicato, Yulanderson Salguero Rodriguez and Paula Daniela Pico Viviescas

In addition to classes and lab projects, students spent the weekends exploring Saudi Arabia at desert camps, cultural events and snorkeling trips. The winter school program was organized by the Visiting Students Research Program (VSRP) team, whose aim is to fulfill KAUST's mission of diversity.

The second Clean Combustion Winter School for graduate and undergrad students will be announced soon at ccws.kaust.edu.sa

The CCRC at the Society of Automotive Engineering 2018 World Congress

Dr. Jean-Baptiste Masurier and Dr. Vallinayagam Raman

The CCRC actively participated in the 2018 Society of Automotive Engineering (SAE) World Congress, in Detroit, Michigan. The three-day event connected talent from academia and industry involved in mobility studies. Attendees shared the latest advances and regulations in automotive science. The CCRC made eight technical presentations in the fields of internal combustion (IC) engine experiments, computational fluid dynamics (CFD) modeling of IC engines and chemical kinetic modeling of gasoline surrogates. Some highlights of these technical presentations included a technique to enable the operation of market gasoline in a partially premixed mode at low loads[1] by CCRC post-doctoral fellow, Raman Vallinayagam. This technique is performed by modifying the engine's valve timing to trap some hot residuals, increasing the reactivity of the fresh charge. Mubarak Ali offered some insight into the super-knock phenomena through computational fluid dynamics[2] by introducing hot spots to the combustion chamber at various initial temperatures, to create end-gas detonation. Mani Sarathy proposed a reduced kinetic model of toluene primary reference fuel, a suitable surrogate to represent a wide spectrum of real fuels[3]. Implementation of the semi-decoupling technique and lumping of species and reactions achieved this reduced kinetic model.

[1] Vallinayagam, R., AlRamadan, A.S., Vedharaj, S., An, Y., et al., Low Load Limit Extension for Gasoline Compression Ignition using Negative Valve Overlap Strategy, SAE Technical Paper 2018-01-0896, 2018, doi:10.4271/2018-01-0896.
[2] Mubarak Ali, M., Hernandez Perez, F., Sow, A., and Im, H., A Computational Study of Abnormal Combustion Characteristics in Spark Ignition Engines, SAE Technical Paper 2018-01-0179, 2018
[3] Sarathy, M., Atef, N., Alfazazi, A., Badra, J., et al., Reduced Gasoline Surrogate (Toluene/n-Heptane/iso-Octane) Chemical Kinetic Model for Compression Ignition Simulations, SAE Technical Paper 2018-01-0191, 2018

KAUST Combustion Institute Summer School

"This school represents combustion research across the globe, which reflects the aim of the Combustion Institute: To encourage global interaction in the field of combustion." Prof. Mani Sarathy, Associate Director, CCRC

Prof. Mani Sarathy , Associate Director, CCRC

During the first week of April, the CCRC hosted the KAUST Combustion Institute Summer School, the first school in the Middle East and North African regions to be sponsored by the Combustion Institute. In this five-day event, distinguished professors and experts in the field of combustion shared their knowledge with students from all over the world. The summer school focused on fundamental combustion in three sessions: flame, engines and fuel, in addition to workshops, networking, and lab demonstrations. More than 80 in-kingdom students, industry participants, and professors, as well as 20 international students, attended the event.

In his opening address, Associate Director of the CCRC, Prof. Mani Sarathy, said "This school represents combustion research across the globe, which reflects the aim of the Combustion Institute: To encourage global interaction in the field of combustion."

Prof. Kaoru Maruta, Tohoku University

In the flame session, Professor Kaoru Maruta, from Tohoku University in Japan, offered an intuitive image of flame fundamentals, introducing experimental phenomena that included flame basics, flammability limits, and flames under extreme conditions, based on experimental methods. KAUST's Hong Im gave a related presentation about fundamental flame theory and its application for practical use. KAUST's Bengt Johansson introduced concepts and applications of internal combustion engines and other low temperature combustion systems in the engine session. Anthony Dean, from GE Global Research, walked his audience through the twentieth century's exciting progress in power generation. He introduced propulsion and power generation in the current context, as well as recent global trends. Finally, he explored the details of combustion.

A gas turbine engine design workshop allowed students to design a small conceptual hybrid-electrical gas turbine. It was a great opportunity for teamwork, using knowledge and rationale to solve practical industrial problems and meet the requirements most students will encounter during their careers.

In the fuel session, KAUST's Aamir Farooq discussed fuel fundamentals based on characterization, experimental chemical kinetics and kinetics diagnostics. Angela Violi, from the University of Michigan, talked about fuel surrogates and the formation of aromatics, PAHs, and soot. Violi said, "From my perspective, the goal of summer school is not only to learn, but to broaden your interests and perhaps explore something different in the future." Students teamed up in the fuel workshop, exploring and designing jet fuel surrogates under realistic situations.

Maryam AlTaher, Saudi Aramco speaks at the panel

The role of women, and their experience in the combustion community was discussed on the last day, at the "Women in Combustion Science" workshop. Maryam AlTaher, from Saudi Aramco, observed that "Humans are capable of bringing value to any discipline, regardless of whether they are male or female. Women are in combustion not to compete, but to complete."

Lectures and workshops from the KAUST Combustion Institute Summer School can be found on YouTube and Facebook.

KAUST Research Conference: Combustion in Extreme Conditions

From March 5 to 8, KAUST hosted industry and academia from across the globe in a conference entitled "Combustion in Extreme Conditions". The conference had three main themes:

- High pressure, high Reynolds number combustion,
- Advanced diagnostics,
- High fidelity, high performance computing.

The conference attracted over 80 visitors. Twenty travel fellowships were awarded to international students traveling from outside of Saudi Arabia.

Dr. James Driscoll, President of the Combustion Institute

Prof. Omer Gülder University of Toronto

The first session of the conference focused on experiments. In the opening keynote address, James Driscoll, current Combustion Institute President said "I believe that KAUST is one of the global centers for combustion research; it's an amazing place and I'm happy for the chance to visit." He went on to discuss premixed turbulent combustion measurements, focusing on extreme turbulence and the need for research beyond the use of simple gases.

Omer Gülder, from the University of Toronto, discussed fundamental studies of soot formation and morphology in laminar co-flow flames at elevated pressures. He shared recent research analyzing soot morphology with transmission electron microscopy and discussed how soot formation changes with pressure.

Dr. Fernando Biagioni GE Power

Prof. Alexei Poludnenko Texas A&M

The two sessions that followed focused on high fidelity, high performance computing. Members from both industry and academia presented research on new and innovative methods of combustion modeling. Fernando Biagioni, from GE Power, discussed some of the challenges in modeling premixed flames in industrial gas turbine combustors. Alexei Poludnenko, from Texas A&M, examined advances in high performance computing and direct numerical simulations that have enhanced our ability to explore combustion problems across timescales of varying magnitude.

Prof. Robert Lucht Purdue University

Dr. Jihad Badra Saudi Aramco

Following the modeling sessions, three more sessions centered on experimental diagnostics, sustainable combustion, and combustion under engine conditions. Purdue's Robert Lucht spoke of the benefits of pulse chirp in femtosecond CARS. Later, Mara de Joannon (CNR, Italy), led a discussion on MILD combustion, and finally, Jihad Badra, from Saudi Aramco, talked about optimizing advanced internal combustion engines. Badra said "Car emission regulations are getting tighter and tighter. The cost of compliance for car companies increases globally with more stringent regulations. Climate, health and energy concerns are among the most pressing issues in the transport sector." The diverse nature of the discussions demonstrated the multi-faceted approach required to overcome the adverse effects of combustion.

Two lab tours demonstrated the world class experimental and computational facilities of the CCRC. CCRC students, post-docs and research scientists presented their studies to visitors. During one of the dinners, students presented their work in a poster session. In the first week of March, 2019, the CCRC will hold a conference on future fuels. Details of this event will be available in our webpage in fall 2018.

Building 7 lab tour

Building 5 lab tour

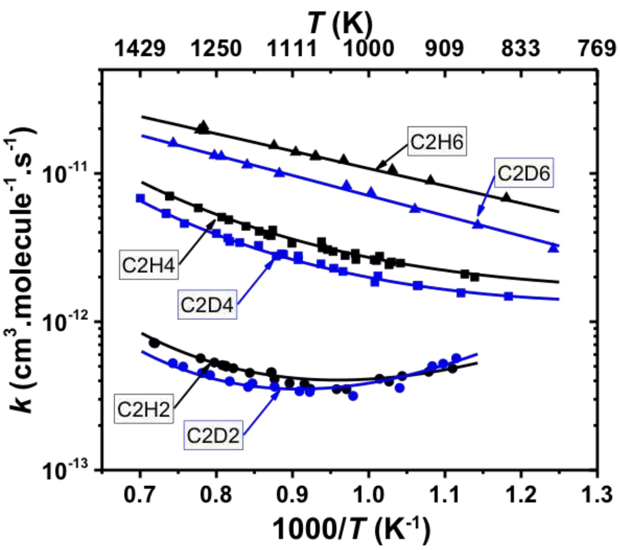
Poster Session

CCRC at the 37th International Symposium on Combustion

It is the goal of the CCRC to be present at key events in the combustion community. At the 37th International Symposium on Combustion, our current research and results will be presented in more than 30 talks, an outline of five such studies follows. Everyone in the combustion community is encouraged to attend in Dublin this summer.

On the reaction of OH radicals with C_2 hydrocarbons

By Fethi Khaled, Binod Raj Giri and Aamir Farooq



Reaction rate of hydroxyl radicals with ethylene, acetylene and their deuterated isotopes

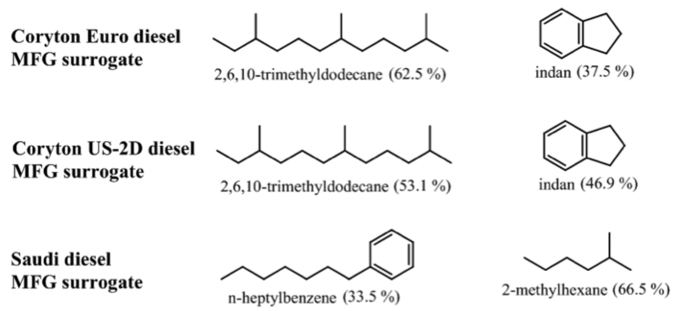
Along with Dr. Binod Raj Giri and Prof. Aamir Farooq (PhD student), Fethi Khaled co-authored a paper on the reaction of unsaturated hydrocarbons (double or triple C-C bond), and hydroxyl radicals (OH). The paper discusses how the addition of OH to the unsaturated C-C bond, and the formation of a relatively stable alcohol adduct, alters the reactivity of these hydrocarbons in a combustion environment. The paper describes the rate of the reaction of OH with the smallest unsaturated hydrocarbons (ethylene, acetylene and their deuterated isotopes), which have been experimentally determined.

The main conclusion of this research is that bimolecular product formation predominates at temperatures T > 850 K for ethylene and T > 1050 K for acetylene. However, at lower temperatures, OH addition to the unsaturated bond is the dominant pathway leading to formation of a stable alcohol adduct (C_2H_4OH and C_2H_2OH), with 100% association at T < 500 K for ethylene, and T < 700 K for acetylene.

These less reactive adducts slow the reactivity of unsaturated hydrocarbons at intermediate to low temperature combustion conditions, as compared to the highly reactive abstraction fuel radicals formed after H-abstraction from saturated hydrocarbons (i.e., alkanes) by combustion radicals that can initiate low temperature combustion pathways by O_2 addition.

Surrogate formulation for diesel and jet fuels using the minimalist functional group (MFG) approach

By Abdul Gani Abdul Jameel, Nimal Naser, Abdul-Hamid Emwas and S. Mani Sarathy



Surrogate species used to represent diesel and jet fuels. Composition (in brackets) in mole %

PhD. student Abdul Gani Abdul Jameel and co-authors Nimal Naser (PhD student), Dr. Abdul-Hamid Emwas (Imaging and Characterization Lab, KAUST), and Prof. Mani Sarathy, have introduced a paper on a new approach for surrogate formulation of real fuels. After formulation of the minimalist functional group (MFG), its efficiency was compared to traditional surrogate formulation methodologies.

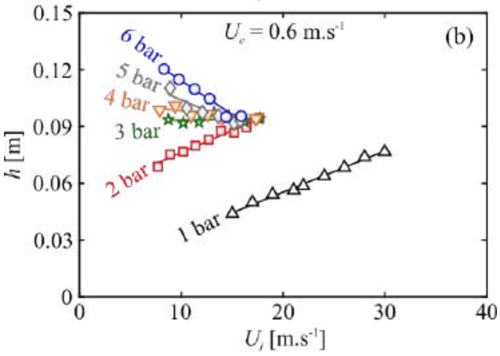
Abdul Gani stressed that simple surrogate mixtures containing as few as two components, and formulated by matching the fuels' functional groups, can reproduce the main combustion properties of real fuels, IQT ignition delay time and derived cetane number (DCN). (A simple surrogate is easier to formulate and test.)

The result was reduced time associated with chemical kinetic mechanism development and lower computational costs for simulations. In this paper, the authors demonstrate the validity of this approach in three practical diesel fuels (Coryton Euro and Coryton US-2D certification grade and Saudi pump grade), and two jet fuels (POSF 4658 and POSF 4734). The functional groups in these fuels were identified and quantified using 1H NMR spectroscopy.

The MFG surrogates also successfully reproduced the fuels' physical and thermochemical properties, including molecular weight, density, H/C ratio and heat of combustion. In addition to its significant scientific results, this paper offers an excellent explanation for 1H NMR spectroscopy and its application in fuel characterization.

Pressure effects and transition in the stabilization mechanism of turbulent lifted flames

By Thibault Guiberti, Wesley Boyette, William Roberts, Assaad Masri



Flame lift-off height as a function of Uj for different pressures and Uc = 0.60 m.s-1

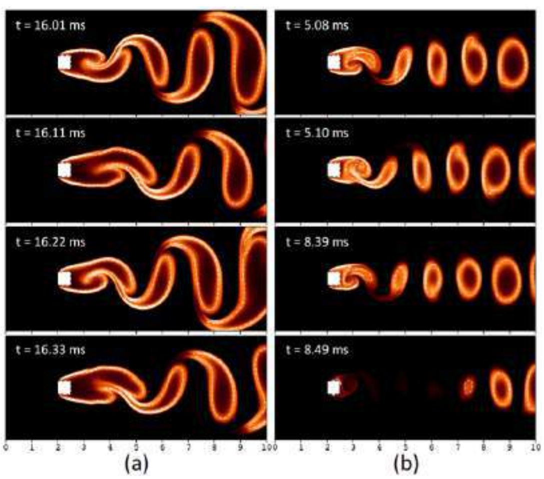
This paper is the result of collaboration among Dr. Thibault Guiberti, Wesley Boyette (PhD student), and Prof. William Roberts, from KAUST, with Prof. Assaad Masri, from the University of Sydney. Thibault and his co-authors have reported measurements at elevated pressures of lift-off and stabilization behavior of turbulent flames, conducted in the state-of-the-art high pressure combustion duct (HPCD) at KAUST.

Lift-off heights were measured from OH*-chemiluminescence imaging, combined with OH relative density and velocity fields, performed using joint OH-PLIF and PIV techniques. These combined diagnostics were used to extract information about the stabilization mechanism. In general, lift-off height increases with pressure and co-flow velocity.

However, this paper highlights the stabilization mechanism of methane flames (as shown previously for ethylene flames), which can transition to a turbulent premixed mode, where the lift-off height decreases with injection velocity, once pressure and co-flow velocity are sufficiently large. This finding confirms that such a transition of the stabilization mode can occur for any fuel, providing specific conditions are met.

Hydrodynamic and Chemical Scaling for Blow-off Dynamics of Lean Premixed Flames Stabilized on a Meso-scale Bluff-body

By Yu Jeong Kim, Bok Jik Lee, Hong G. Im



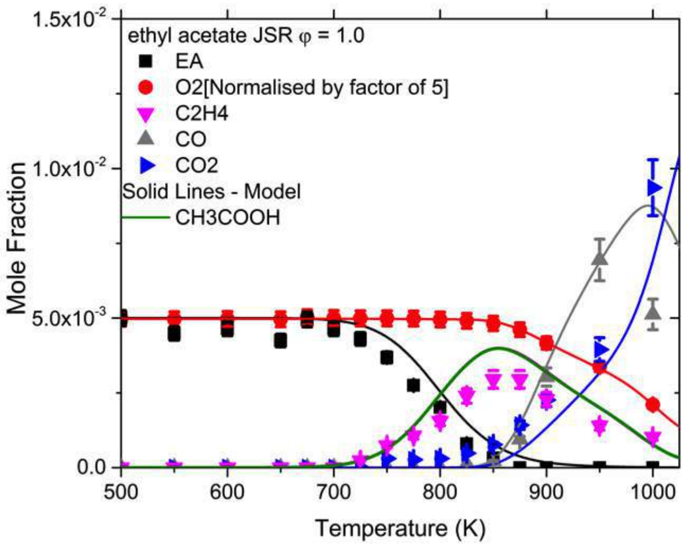
Isocontour of heat release rate in hydrogen-air mixtures for case at Φ= 0.5, Tin = 500 K: (a) The transient event at U = 65 m/s and (b) Blow-off event at U = 73.6 m/s.

PhD. student Yu Jeong Kim, with Dr. Bok Jik Lee from the Gwangju Institute of Science and Technology in Korea, and Prof. Hong G. Im, have co-authored this paper. It focuses on direct numerical simulations (DNS) of the effect of density ratio between burned and unburned regions and laminar flame speed on the conditions of the onset of local extinction and blow-off of lean premixed hydrogen-air and syngas-air flames.

A lower density ratio was found to promote extinction with a scaling factor--the Strouhal number. It was also found that the condition for the onset of local extinction and blow-off was dictated largely by the competition between flow residence time and ignition delay of the local mixtures scaled by the Damköhler number. The paper also reports good simulated images of flame dynamics during its transition towards extinction.

Small Ester Combustion Chemistry: Computational Kinetics and Experimental Study of Methyl Acetate and Ethyl Acetate

By Ahfaz Ahmed, William J. Pitz, Carlo Cavallotti, Marco Mehl, Nitin Lokachari, Elna J.K. Nilsson, Jui-Yang Wang, Alexander A. Konnov, Scott W. Wagnon, Bingjie Chen, Zhandong Wang, Henry J. Curran, Stephen J. Klippenstein, William L. Roberts, S. Mani Sarathy



JSR measurements (symbols) for EA oxidation and predictions (lines) with the kinetic model

A group study combining experimental and theoretical investigations will be presented at the 37th International Symposium on Combustion by PhD student Ahfaz Ahmed. The impressive list of co-authors demonstrates the importance of the CCRC's international collaborations.

This paper details the development of a comprehensive kinetic model for methyl acetate and ethyl acetate, both favored fuels for advanced spark ignition engines. To thoroughly validate the model, wide ranging investigations were conducted which included speciation measurements, detailed quantum chemistry calculations, chemical ignition delay times and flame speed measurements.

The study is a comprehensive tutorial on how a detailed kinetic model can be built for a novel fuel by joining different theoretical and experimental capabilities and the combined efforts of scientists in the wider combustion community. This paper is expected to be a major contribution, and a highly cited work of the alternate fuels era.

KAUST – Boeing collaborative research

Ariff Magdoom Mahuthannan and Dr. Peng Liu

The Clean Combustion Research Center and the Boeing Company have collaborated on research projects since May 2015. The context of these projects is aircraft fire and explosion hazards; and their main objective is to provide a better understanding of the mechanisms involved during these dramatics events. Specifically, in two ongoing projects "Characterization of flame quenching processes in combustion arresters" and "Radio frequency ignition hazard", groups headed by William Roberts and Deanna Lacoste will investigate how new materials and new sensors can change ignition and fire propagation threats in aircraft.

Flame quenching processes in combustion arresters

"After designing and building a lab scale experimental model of combustion arresters used in aircraft fuel tanks, we identified one of the most important parameters affecting the quenching process--the propagation speed of the combustion front", explained Prof. Roberts. "Keeping all the other parameters constant (fuel, equivalence ratio, pressure, etc.), the speed of the flame can change the quenching distance by more than a factor of two. This was a new result; and with Eddie Kwon and Jason Damazo from the Boeing Company, we decided to focus on understanding this velocity effect", he said.

To reach this goal, Dr. Peng Liu (post-doctoral fellow), and Ariff Magdoom Mahuthannan (PhD student), are performing measurements with an advanced optical diagnostic that allows simultaneous measurements of the temperature field and the hydroxyl (OH) radical density during quenching events. This technique, called two-color planar laser induced fluorescence, has been validated for numerous combustion configurations, but it remains a challenge to implement in a constant volume combustion chamber, for which single shot measurements are necessary.

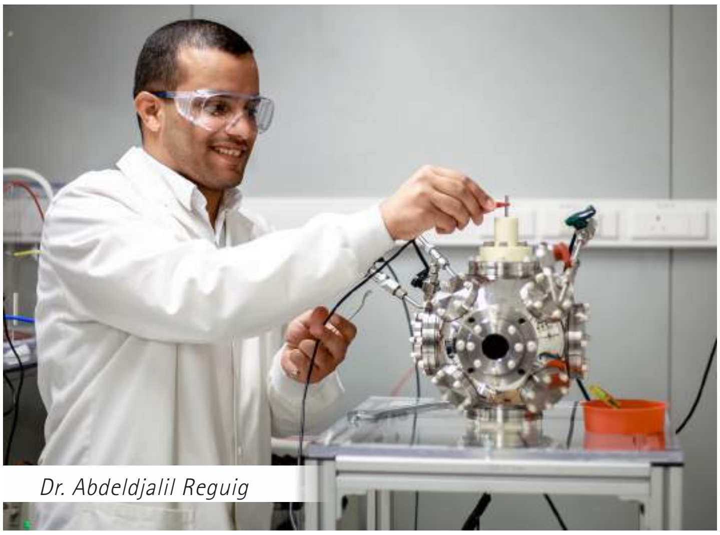
"The current results are promising and we hope that in the coming months, we can propose a model of the effect of the flame velocity on heat transfer and radical quenching by the surface", said Ariff Magdoom.

Radio frequency ignition hazard

"Wireless communication between different devices is not neutral in terms of the ignition hazard. For example, wireless sensors transmit data via radio frequency (RF) signals, and under certain conditions, RF signals can ignite combustible mixtures", Prof. Lacoste explained.

The aim of this project is to better characterize the ignition threat by RF electric fields, under conditions relevant for aircraft safety, i.e., for gas pressure ranging from 0.1 to 1 bar. This research, started in March 2018, will be a combination of experimental and analytical investigations. In collaboration with Eddie Kwon and Jason Damazo, the design of the experimental setup is nearly complete.

Post-doctoral fellow Abdeldjalil Reguig is currently building the ignition cell. The objective, within two years, is to characterize ignition hazard for a large range of RF signals and to provide a data base and a comprehensive model that could be used for validation of numerical simulations and for the extrapolation to other conditions.



Dr. Abdeldjalil Reguig

Post-doc opportunities at CCRC

Development of sensitive absorption diagnostics based on cavity-enhanced multi-heterodyne spectroscopy in the mid-infrared

Duration one year, extendible for two years.

Seeking applicants with a PhD degree and strong background in one or more of the following: optical diagnostics / laser-based sensors / non-linear optical methods / cavity-enhanced spectroscopy / frequency-comb spectroscopy. For questions or an application, contact Prof. Aamir Farooq, aamir.farooq@kaust.edu.sa

Experimental and modelling study of heterogeneous chemistry for catalyst-based exhaust after-treatment systems.

Duration one year, extendible for two years.

Seeking applicants with a PhD degree and a strong background in one or more of these areas: experimental methods for heterogeneous chemistry / modelling of gas-solid reactions / synthesis of catalytic materials / design of after-treatment systems. For questions or an application, contact Prof. Aamir Farooq, aamir.farooq@kaust.edu.sa

Experimental study of efficient and scalable methods for nanomaterial synthesis through combustion- and plasma-based techniques.

Duration one year, extendible for two years.

Seeking applicants with a PhD degree in combustion science or plasma physics and up to three years research experience after PhD graduation. Applicant should have strong experimental background in combustion, or plasma discharges at atmospheric pressures. Expertise in synthesis of nanoparticles will be an asset. For questions or an application, contact Prof. Lacoste: deanna.lacoste@kaust.edu.sa

Experimental investigation of oxy-fuel combustion with CO2 dilution under gas turbine conditions.

Duration one year, extendible for two years.

We are seeking applicants with a PhD in mechanical, aerospace engineering or combustion science, or other relevant disciplines, with up to three years of experience after a PhD. Strong experimental background and experience in combustion is required. Experience with design and operation of high pressure burners, and laser diagnostics is highly desirable. For questions or for an application, contact Prof. Magnotti: gaetano.magnotti@kaust.edu.sa

Development of advanced laser diagnostics for high-pressure combustion.

Duration one year, extendible for two years.

Seeking applicants with a PhD in applied physics, mechanical, aerospace engineering, combustion science or other relevant disciplines, with up to three years of experience after a PhD. Strong experimental background and experience in laser diagnostics' development is required. Experience in combustion, pulse-burst lasers or picosecond lasers is highly desirable. For questions or an application, contact Prof. Magnotti: gaetano.magnotti@kaust.edu.sa

Combining Chemical Kinetics and Machine Learning to Predict Complex Reaction Networks.

Duration one year, extendible for two years.

The goal is to improve combustion engines and industrial chemical reactors with detailed understanding of complex chemical reaction networks. We are seeking an individual with expertise in chemical reaction engineering, combustion, and kinetics. Expertise in artificial neural networks and genetic algorithms is also required to predict a wide range of combustion properties using a limited number of input parameters. The applications of machine learning will be extended to predict important thermochemical and kinetic properties of reacting systems using quantum mechanical properties of the fuel and combustion intermediates (e.g., electronic structures and stationary point energies). Contact Prof. Sarathy: mani.sarathy@kaust.edu.sa

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