جامعة الملك عبدالله
للعلوم والتقنية
King Abdullah University of
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KAUST
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CCRC Clean Combustion Research Center

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Reactive Flow Modeling Laboratory
KAUST Future Fuels Workshop
36th Int'l Symposium on Combustion

CREDITS

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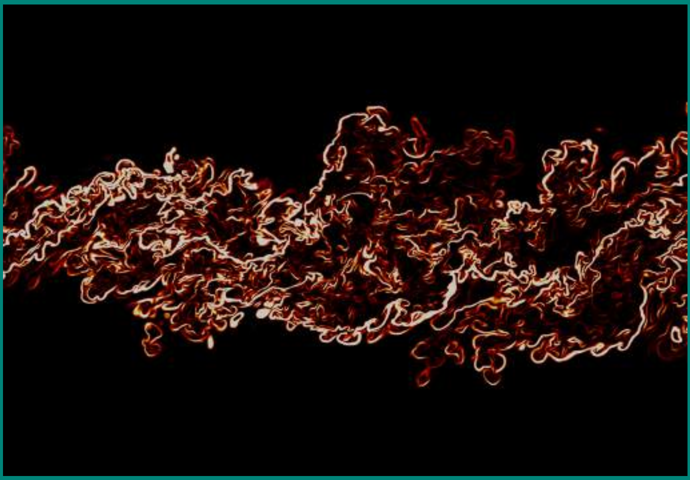
Reactive Flow Modeling Laboratory



Scalar dissipation rate field in a turbulent mixing layer at high Reynolds number (A. Attili and F. Bisetti, Phys Fluids 24, 2012; Phys Rev E 88, 2013)

Fabrizio Bisetti is one of the CCRC's founding faculty members, having joined KAUST in the Fall of 2009. Initially, the Reactive Flow Modeling Laboratory (RFML) included two post-docs and two students. During his seven years at KAUST Dr. Bisetti supervised and managed 14 students, 12 post docs, and one research scientist. He established a world class research program in combustion, turbulence, and large scale computing, with a focus on fundamental and applied challenges in simulating complex reactive flow problems.

Dr. Bisetti and his team made substantial contributions in many areas of fluid dynamics and combustion. His work on the simulation of soot formation in turbulent flames represents the state-of-the-art in the direct numerical simulation of these complex multi-physics phenomena, and helped to shed light on the complex interaction between soot formation, chemistry, and turbulence. His team also investigated the formation and growth of liquid aerosols in laminar and turbulent flows, performing several detailed simulations and experiments.

During his years at KAUST, Dr. Bisetti developed an interest in plasma chemistry and physics and electric field-assisted combustion. He developed elementary models for simulating electrons and ions, which have been applied to replicate the current drawn from laminar flames subject to bias voltage.

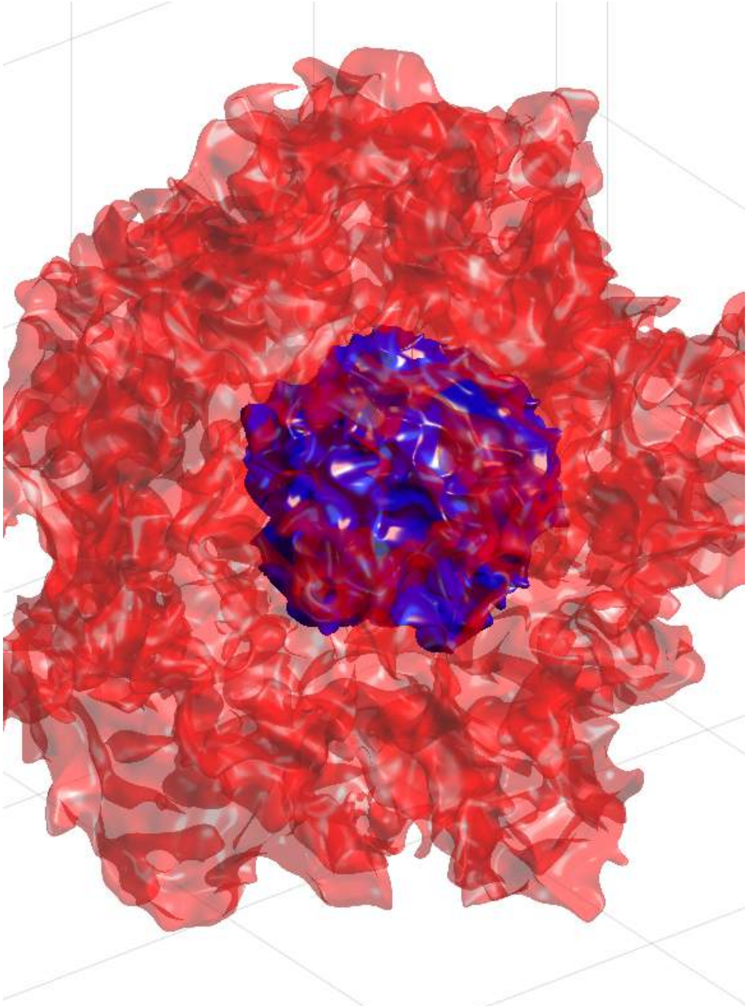
Most of Dr. Bisetti's work is based on very large scale and massively parallel simulations. His team members have been among the most active users of the unique computational facilities available at KAUST, Shaheen I and II. This interest in extreme computing has led to some of the largest simulations of turbulence and combustion in KAUST--and in the world-- including a series of simulations of turbulent mixing layers which reached a Reynolds number never before achieved. Recently, Fabrizio and his team started a project on turbulent premixed flames that featured massively parallel simulations of methane/air combustion, using up to 20 billion grid points and 16 chemical species. This unprecedented set of simulations will contribute to the understanding of the long standing problem of flame propagation in turbulent flows.

The unique databases produced by Bisetti's team are made available to the combustion and fluid dynamics communities, and have been used by many leading institutions and researchers throughout the world.

Dr. Bisetti played a critical role in the development of the Mechanical Engineering curriculum at KAUST. During his seven years, he taught graduate level courses in thermodynamics, fluid mechanics, turbulence, turbulent combustion, and computational fluid dynamics. His philosophy of the quantum foundations of thermodynamic concepts is a popular example of the in-depth knowledge admired by his students, and his outstanding mathematical perceptions challenge common comprehension of the derivation of equations and their routine application.

Dr. Bisetti will take a position in the Department of Aerospace Engineering and Engineering Mechanics at the University of Texas at Austin. He takes with him our very best wishes for his continued success.

A key member of the RFML team is Research Scientist Antonio Attili, who will soon join RWTH Aachen University in Germany. During his time at KAUST, Dr. Attili demonstrated his excellence as a teacher and mentor. Among his very many contributions to the research of the RFML is his interest in laminar and turbulent combustion, which emphasizes the role of hydrodynamic and scalar transport, in addition to reaction kinetics. In so doing, his work has encouraged novel and insightful research into known flame mechanisms. Attili's energy in working with students has promoted excellent standards in academic publishing. In 2015, he taught an advanced level course on turbulent mixing in which he discussed, in unprecedented detail, the ubiquitous nature of turbulent mixing processes, the fundamental equations used to model turbulence, and the statistical methods needed to understand its randomness.



Visualization from a Direct Numerical Simulation of a spherical expanding turbulent methane flame at 4 atm (simulation performed by R. Buttay, S. Luca, A. Attili, F. Bisetti)

The FUTURE FUELS WORKSHOP encompasses a wide spectrum of cutting edge technologies relevant to fuel production, utilization and global sustainability issues with an emphasis on low-grade and alternative fuels for transportation, and stationary power generation.

KAUST FUTURE FUELS WORKSHOP

#Destination KAUST

The KAUST 2016 Future Fuels Workshop was organized by the CCRC and co-chaired by William Roberts, Hong Im and Aamir Farooq. The workshop joined international experts from academia, national laboratories, and industry, who shared their vision for energy in fuel sustainability, production, utilization and chemistry, as well as the use of low-grade fuels. The workshop promoted international collaborations focusing on fuel formulation and utilization of clean and efficient energy systems. The event attracted 100 researchers from 20 countries.

Opening remarks were delivered by Yves Gnanou, Dean of Physical Science and Engineering at KAUST, William Roberts, Director of CCRC KAUST, and Ahmed Al Khowaiter, CTO of Saudi Aramco. Five topics were covered in five sessions during the workshop.

The Fuel Sustainability Session was chaired by Bengt Johansson (KAUST). Tadeusz Patzek, also from KAUST, discussed the unsustainability of fuel and energy systems, emphasizing the reasons why major fuel systems--including biofuels--are fundamentally unsustainable. Amer Amer, from Saudi Aramco, discussed the flexibility of fossil-based fuels for maximizing environmental benefits by deploying sustainable mobility solutions such as co-optimization of fuel and engine systems. Robert Kee (Colorado School of Mines) discussed increasing the role of natural gas for energy generation and improvement of the Fischer-Tropsch process to enhance its utility by gas-to-liquid conversion. Jay Gore (Purdue) examined sustainable recycling of CO_2 to hydrocarbons by solar energy and catalysis.

The Fuel Production Session was chaired by KAUST's Mani Sarathy. Blake Simmons (JBEI), highlighted potential challenges and solutions in the production of biofuels from non-food lignocellulosic biomass. George Huber, of the University of Wisconsin-Madison, gave a comprehensive overview of recent pioneering biofuel startups, and attributed their failure to underpredicted economic estimates and pilot plants operating at low capacities.

Min Suk Cha (KAUST) presented his research on reformed liquid fuel production using electrical discharge reactors. John Benemann, from MicroBio Engineering, offered evidence for the economic impracticality of biofuel production using algae. Kevin Van Geem (Ghent University) considered clean fuel production via biomass fast pyrolysis.

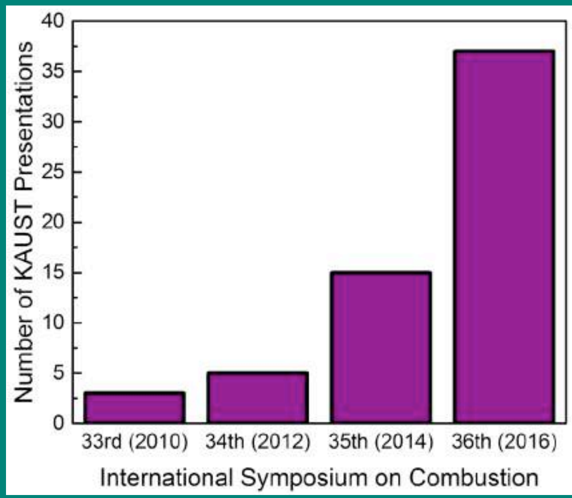
The Fuel Utilization Session was chaired by Robert Dibble from KAUST. Robert McCormick (NREL), emphasized relations between chemical structures and relevant fuel properties for optimizing engine performance, with a perspective on biofuels. GE's Jeffrey Goldmeer discussed challenges and opportunities in utilizing fuels for power generation--including gas and crude oil. Bengt Johansson from KAUST offered several approaches to improving engine efficiency by employing higher compression ratio, friction reduction and improved gas exchange. Jenny Larfeldt (Siemens) considered the benefits and challenges associated with fuel flexible turbines. SukHo Chung (KAUST) examined the effects of fuel on soot formation; results for gasoline surrogates and simpler molecules were presented. Olaf Deutschmann (Karlsruhe Institute of Technology) provided an overview on state-of-the-art exhaust-gas after-treatment devices and current technological trends. Saudi Aramco's Kai Morganti highlighted synergistic co-development of engine/fuel systems to power future combustion engines for reduced emissions and improved fuel efficiency.

The Fuel Chemistry Session was chaired by Hong G. Im, from KAUST. Uwe Reidel, of the German Aerospace Center, posed several questions on how the composition of alternative jet fuels affects thermo-physical and thermo-chemical properties, as well as the combustion characteristics. Tiziano Faravelli (Politecnico di Milano) examined the challenges of developing chemical kinetic mechanisms for oxygenated fuels. Aamir Farooq (KAUST) presented his research on fundamental experiments (ignition, speciation, and rate measurements) of future fuels. Angela Violi, from the University of Michigan, discussed several aspects of conventional and alternative fuels, including surrogate formulation, mechanisms of nanoparticle formation, and the health effects associated with these nanoparticles. KAUST's Mani Sarathy presented a simulation-based fuel/engine design methodology based on first principles.

The Low Grade Fuels Session focused on heavy fuel oils (HFOs) and naphthas; it was chaired by Aamir Farooq from KAUST. The keynote lecture on combustion and emissions properties of HFOs was delivered by Princeton's Frederick Dryer. Predictive simulations of low grade fuel combustion in laboratory scale combustors were discussed by Hong Im from KAUST; and Christian Hasse from the Technische Universität Bergakademie Freiberg presented several energetic and non-energetic uses for low-grade fuels. Bill Roberts discussed cenosphere formation in HFO combustion, which increase boiler maintenance costs, decrease combustion efficiency, and violate current emission regulations.

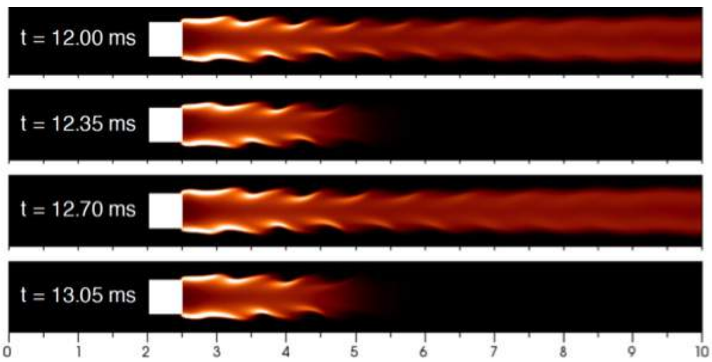
36th Int'l Symposium on Combustion

Every two years, the International Symposium on Combustion presents the most advanced research in 14 areas in its field. At the 33rd International Symposium on Combustion in 2010, KAUST made its debut with three presentations. This year, 37 studies performed at KAUST, or in collaboration with KAUST researchers, will be presented at the 36th International Symposium on Combustion in South Korea. Abstracts from three of those papers are presented here.



DYNAMICS OF BLUFF-BODY STABILIZED LEAN PREMIXED SYNGAS FLAMES IN A MESO-SCALE CHANNEL

B.J. Lee, H.G. Im
(For presentation at the Laminar Flames colloquium)



Temporal sequence of heat release rate isocontours for the syngas flames at U = 16.7 m/s, showing a periodic oscillation mode.

Direct numerical simulations were conducted to investigate the dynamics of lean premixed syngas flames stabilized by a bluff body in a meso-scale channel at near blow off conditions to provide fundamental insights into the physical mechanisms responsible for the critical phenomena.

Flames in a two-dimensional meso-scale channel with a square flame holder were adopted as the model configuration, and a syngas mixture at an equivalence ratio of 0.5 with the CO:H_2 ratio of 1 were considered.

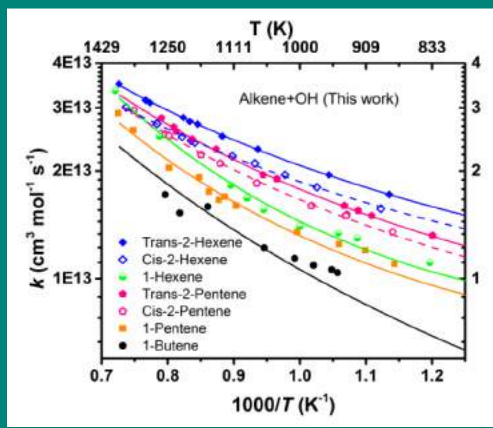
As the inlet velocity was increased, the initially stable steady flames underwent a transition to an unsteady mode of regular asymmetric fluctuation. When the inlet velocity was further increased, the flame was eventually blown off.

Between the regular fluctuation mode and the blow off limit, a narrow range of the inlet velocity existed where the flames exhibited periodic local extinction and recovery. Approaching further to the blow off limit, the recovery mode failed to occur, but the flame survived as a short kernel attached to the base of the bluff body, until it was completely extinguished as the attached flames were gradually shrunk towards the bluff body.

The results were systematically compared with the hydrogen flame results reported in an earlier study by this group. Examination of the characteristic time scales of relevant processes provided an understanding of key mechanisms responsible for the observed differences, thereby allowing improved description of the local extinction and re-ignition dynamics that are critical to flame stabilization.

A SHOCK TUBE STUDY OF C4 - C6 STRAIGHT CHAIN ALKENES + OH REACTIONS

F. Khaled, J. Badra, A. Farooq
(For presentation at the Reaction Kinetics colloquium)



Rate coefficient of reaction of C4, C5 and C6 alkenes with OH radicals. Lines represent curve fits to data.

Alkenes are known to be good octane boosters and major components in commercial fuels. Detailed theoretical calculations and direct kinetic measurements of elementary reactions of alkenes with combustion radicals are scarce for C4 alkenes, and nearly absent for C5 and larger alkenes.

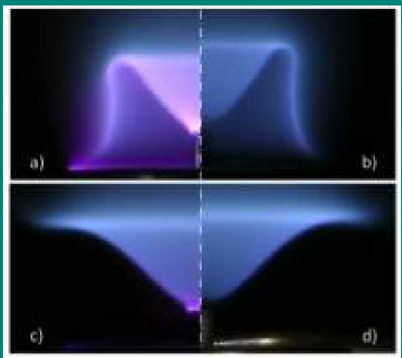
Shock tube used to measure reaction rates

The overall rate coefficients for the reaction of OH radical with 1-butene (CH_2=CH-CH_2-CH_3, k_I), 1-pentene (CH_2=CH-CH_2-CH_2-CH_3, k_{II}), cis/trans 2-pentene (CH_3-CH=CH-CH_2-CH_3, k_{III} and k_{IV}), 1-hexene (CH_2=CH-CH_2-CH_2-CH_2-CH_3, k_V) and cis/trans 2-hexene (CH_3-CH=CH-CH_2-CH_2-CH_3, k_{VI} and k_{VII}) were measured behind reflected shock waves over a temperature range of 833 – 1377 K and pressures near 1.5 atm.

Reaction progress was followed by measuring the mole fraction of OH radicals near 306.7 nm using a UV laser absorption technique. It was found that the rate coefficients of OH + trans-2-alkenes were larger than those of OH + cis-2-alkenes, followed by OH + 1-alkenes. The derived Arrhenius expressions for the overall rate coefficients (in $cm^3.mol^{-1}.s^{-1}$) are given in the paper.

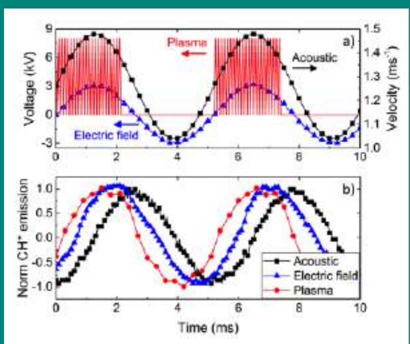
TRANSFER FUNCTIONS OF LAMINAR PREMIXED FLAMES SUBJECTED TO FORCING BY ACOUSTIC WAVES, AC ELECTRIC FIELDS, AND NON-THERMAL PLASMA DISCHARGES

D.A. Lacoste, Y. Xiong, J.P. Moeck, S.H. Chung, W.L. Roberts, M.S. Cha
(For presentation at the Novel Combustion Concepts, Technologies and Systems colloquium)



Methane-air M- and V-flames (b) & (d), forced by non-thermal plasma discharges (a) & (c)

The response of laminar methane-air flames to forcing by acoustic waves, AC electric fields, and nanosecond repetitively pulsed (NRP) glow discharges are reported here. The experimental model consisted of an axisymmetric burner with a nozzle made from a quartz tube.



Forcing signals at 196 Hz and corresponding temporal evolution of normalized CH emission of M-flame.*

Three different flame geometries were studied: conical, M-shaped and V-shaped flames. A central stainless steel rod was used as a cathode for the electric field and plasma excitations. The acoustic forcing was obtained using a loudspeaker located at the bottom of the burner. For forcing by AC electric fields, a metallic grid was placed above the rod and connected to an AC power supply.

Plasma forcing was obtained by applying high voltage pulses of 10-ns duration at 10 kHz, between the rod and an annular stainless steel ring, placed at the outlet of the quartz tube. For forcing by acoustic waves and plasma, the geometry of the flame plays a key role in the response of the combustion, while flame shape does not affect the response of the combustion to electric field forcing. Flame response to acoustic forcing of about 10% of the incoming flow is similar to that obtained in the literature.

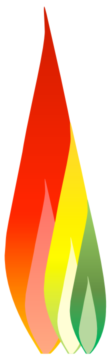
Flames were responsive to an AC electric field across the entire range of frequencies studied. A forcing mechanism, based on the generation of ionic wind, is proposed. The gain of transfer function obtained for plasma forcing was found to be as much as five times higher than for acoustic forcing. A possible mechanism of plasma forcing is introduced.

CCRC Images

The design symbolizes a tall and vigorous tree, a source of clean and efficient power, blossoming in colors that represent the main branches of CCRC research, experimentation, simulation, and chemical kinetics. At its core, a flame burns under a conical flask, representing the combustion that is the core interest at the Center, and resulting in major involvement in the oil, automotive, and aeronautics industries. From its branches, extend CCRC's contributions to clean energy, the environment, oil economy, human health, and knowledge.

Under the tree are buildings that represent the physical presence of KAUST and CCRC research; two smaller trees suggest that CCRC leads and cultivates the field of environmental study. The exuberant foliage--the colors of KAUST's logo--symbolizes CCRC's rapid growth as a leader in the field of combustion.

This design was created by Penghui Cheng, MS student in the CCRC.
Made with http://logomakr.com (Logo Maker).



The goal of the CCRC is to be a leader in the development of combustion technologies that reduce emissions and increase combustion efficiency.

A series of flame kernels transition from dark red to yellow to green, diminishing as they move from left to right. The larger, dark red color represents the current stage of combustion technology with high emissions and low efficiency. Yellow is the transition to more efficient combustion technology with lower emissions and greater efficiency; and the last flame kernel, in green, represents the ultimate goal--combustion technology that enables the lowest emissions and the greatest efficiency, reflecting the objectives of the Clean Combustion Research Center of KAUST.

This design was created by Awad Alquaity, PhD student in the CCRC

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