Combustion to Enable an Efficient Future

SEVENTH SAUDI ARABIAN SECTION OF THE COMBUSTION INSTITUTE ANNUAL MEETING

King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

May 21 – 22, 2017
Welcome to SAS-CI 2017

Welcome to the Seventh Annual Meeting of the Saudi Arabian Section of the Combustion Institute (SAS-CI). Under the theme of “Combustion to Enable an Efficient Future” this year’s event brings together more than 100 researchers from various institutions in and out of the Kingdom of Saudi Arabia.

In its short history, the Saudi Arabian Section has grown in both size and stature. The Section currently has more than 134 registered members. But more importantly, our Annual Meeting has also been attracting an increasing number of national researchers with each passing year with better involvement from KAUST, Saudi Aramco, KFUPM, KACST, KAPSARC, KAU, Royal Commission of Yanbu Research Center, Taif University, Taibah University, Jubail University College and Prince Mohammed Bin Fahad University. This reflects favorably upon the standard of research undertaken within our local community. We expect that the national and international participation rate will continue its upward trajectory in future years, with our 2017 submissions also featuring co-authors from research groups based in, Saudi Arabia, United States, Korea, Malaysia, Egypt, Emirates, Algeria, United Kingdom, Ireland, Australia, and Turkey.

The Seventh Annual Meeting is hosted by King Abdullah University of Science and Technology in Thuwal. Collectively, the meeting will feature four invited lectures, 39 oral presentations across four different technical sessions and 20 poster presentations.

Welcome and we hope that you enjoy the Seventh Annual Meeting.

The Seventh Annual Meeting Organizers are

Maryam Altaher
Saudi Aramco

Jihad Badra
Saudi Aramco

Louise Belanger
KAUST

Raheena Abdurehim
KAUST

Thanks also extend to

Ibrahim Algunaibet
Saudi Aramco

Husain Baaqel
Saudi Aramco

Abdullah Alramadan
KAUST
THE COMBUSTION INSTITUTE

SAUDI ARABIAN SECTION

Section Leadership

Chairman  Dr. Amer Amer  Saudi Aramco
Vice-Chairman  Prof. William Roberts  KAUST
Vice-Chairman  Dr. Ahmed Al-Harbi  KACST
Secretary  Dr. Jihad Badra  Saudi Aramco
Officers
Dr. Kai Morganti  Saudi Aramco
Prof. S. Mani Sarathy  KAUST
Prof. Nadeem Malik  KFUPM
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<td><strong>Session Chair: Nicholas Chase</strong>, KAPSARC, KSA</td>
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<td>“Oil Refining in a CO₂ Constrained World: Implications for Transport Fuels Policymaking”</td>
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# Meeting Agenda and Oral Presentations - Monday May 22\textsuperscript{nd}

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**Jihad Badra**  
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| 6:45 – 8:45 | **DINNER AT ISLAND RECREATION CENTER** |
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1st Invited Speaker

Energy Demand in the Transportation Sector

Nicholas Chase
Transportation and Urban Infrastructure Team
King Abdullah Petroleum Studies and Research Center (KAPSARC)
nicholas.chase@kapsarc.org

The transportation sector today accounts for about one-quarter of the world’s delivered energy consumption and a similar share of energy-related greenhouse gas (GHG) emissions. It is also the single largest end-use consumer of petroleum products. Looking ahead, the transportation sector may be on the cusp of significant changes that could dramatically impact future energy markets. First, surging demand for transportation in emerging economies has reshaped the geography of energy consumption away from industrialized economies and towards much more populous regions where passenger and freight demand could continue to grow rapidly. This is especially true to the two emerging energy giants—China and India. How will this geographic change continue into the future? Further, transportation energy demand is expected to undergo change in other dimensions. The modal distribution and consequently the types of fuels consumed are widely expected to change from today. Rapid developments are taking place across areas such as new energy efficient technologies, greater use of non-petroleum fuels for motive power, and new travel demand paradigms through concepts such as shared mobility. The impact of these developments on global transportation energy demand are uncertain but have the potential to greatly change future energy markets and the environment. How can these developments shape the future of global transportation energy demand?

The relationship between transportation energy demand per capita and Gross Domestic Product per capita, 1971-2014

![Graph showing the relationship between transportation energy demand per capita and Gross Domestic Product per capita, 1971-2014.](image-url)
Biography

Nicholas is a Research Fellow at the King Abdullah Petroleum Studies and Research Center (KAPSARC) on the Transportation and Urban Infrastructure Team. His research explores the future of transportation energy demand in China and India, specifically looking at the energy demand in the movement of freight as well as the potential for LNG as a maritime and waterway fuel in China. Previous to KAPSARC, Nicholas was an economist and transportation energy demand modeller at the U.S. Energy Information Administration at the U.S. Department of Energy. He did his undergraduate work at the University of Michigan-Ann Arbor and his graduate work at Johns Hopkins University.
2nd Invited Speaker

Compositional Inhomogeneties in Turbulent Flames

Prof. Assaad R. Masri
School of Aerospace, Mechanical and Mechatronic Engineering
The University of Sydney, Australia
assaad.masri@sydney.edu.au

Compositional inhomogeneity which is quite a common feature of practical combustion systems, may be either intentionally introduced such as in stratified engines or may be induced by virtue of system instabilities such as lean premixed gas turbines. In either cases, mixed-mode combustion prevails where reaction zones may transition from fully non-premixed, to stratified and premixed flames. Understanding the flame structure as it transitions through these modes has only recently started to unfold. More importantly, the ability to model such flames remains a challenge as numerical approaches are generally not well-equipped to cope with multi-modes of burning and it is only recently that reliable data has become available for model validation.

The presentation will review recent advances in this field with a particular focus on the Sydney piloted burner with compositionally inhomogeneous inlets. This burner was recently introduced as an ideal platform featuring mixed-modes of combustion and showing enhanced stability with varying gradients of mixture fraction at the inlet. This and other characteristics of the flames with enhanced stability are now a challenge to modellers worldwide. The following aspects of the flames stabilised on this new burner will be addressed during the talk: (i) effects of fuel reactivity on stability, (ii) statistics of scalar dissipation rates and reaction progress variables, (iii) lean modes of combustion, (iv) projected effects of high pressure on turbulent mixing and flame stability, and (v) recent advances in modelling mixed-modes of combustion.

Fig.1 Reaction progress variable versus mixture fraction measured at various axial location in a homogeneous (Lr=300) and three inhomogeneous flames (Lr75) flames with jet velocities increasing from 57m/s to 80m/s and 103m/s (bottom row).
Biography

Masri has received his PhD (1987) and BE Honours with the University Medal (1984) from the University of Sydney. He is currently a Professor in the School of Aerospace, Mechanical and Mechatronic Engineering, Faculty of Engineering and Information Technologies at the University of Sydney and Chairman of the Australia and New Zealand section of the Combustion Institute. Masri’s research lies in the broad area of efficient energy conversion with a focus on turbulent combustion of gaseous and liquid fuels and laser diagnostics. His current research areas include: combustion of bio-fuels and biodiesels, atomization of sprays, turbulent inhomogeneous flames, explosion and industrial safety and nanoparticle formation in flames. Masri has published over 130 journal papers and won many awards including the Silver Medal of the Combustion Institute. He was recently co-chair of the prestigious 36th International Combustion Symposium which took place in Seoul, August 2016.
3rd Invited Speaker

Recent Trends in CO₂ Capture and Utilization Technologies

Dr. Aqil Jamal

Carbon Management R&D Division, Saudi Aramco Research and Development Center, Saudi Arabia
aqil.jamal@aramco.com

Carbon Capture, Utilization and Storage (CCUS) is a key technology platform to enable deep reduction of greenhouse gases while meeting the growing global energy demand. Power plant and process industries are the two biggest sectors where large amounts of CO₂ can be captured in a cost-effective manner for further utilization or underground storage. Recent advances in material science offer new opportunities for economically feasible CO₂ capture and utilization in combination with renewable energy. This presentation will cover innovative materials and approaches to capture and utilize CO₂ from industrial point sources and highlight key carbon capture and utilization technologies under development at Saudi Aramco.
Biography

Dr. Aqil Jamal is the Chief Technologist leading the Carbon Management Research Division of Saudi Aramco’s R&D Center in Dhahran. Dr. Jamal is responsible for directing research in Carbon Capture and Utilization, Energy Efficiency and Renewables. Prior to joining Saudi Aramco, Dr. Jamal has been involved in process development research related to carbon capture and utilization, energy conversion, gasification and hydrogen production areas. Also, before joining Saudi Aramco Dr. Jamal has worked in various capacities with Fluor Corp., Praxair and RTI International. Dr. Jamal holds a Ph.D. degree in chemical engineering from the University of British Columbia and did his post-doc research with National Energy Technology Lab (NETL), U.S. DOE, in Pittsburgh PA.
Effects of Flow Turbulence and Fuel Type on the Structure and Blowoff Characteristics of Bluff-Body Stabilized Lean Premixed Flames

Prof. Baki M. Cetegen

Department of Mechanical Engineering
University of Connecticut, Storrs, CT
baki.cetegen@uconn.edu

The structure of unconfined, lean premixed, bluff body stabilized flames is studied for different levels of turbulence intensity in the approach flow and different fuels (methane, propane, ethylene). The mixture approach velocities range from 5 to 15 m/s while the mean turbulence intensity levels between 4 and 30 % are achieved by using suitable turbulence generation schemes. These conditions allow reaching turbulence Reynolds numbers, based on the fluctuating velocity and turbulence integral length scale, of up to 8000. Planar laser induced fluorescence (PLIF) of OH and CH$_2$O and particle image velocimetry (PIV) are performed for simultaneous heat release and velocity measurements. The flame structure is observed to be strongly modified by the turbulent flow field. Formation of cusps and unburnt mixture fingers are observed as the turbulence intensity is increased from 4 to 14 %, but for these cases the heat release front remains continuous. For turbulent conditions higher than 14 % rms, localized extinctions occur along the flame surface creating isolated pockets of OH with heat release occurring along its boundary. Pockets of preheated reactants along with fresh reactants are also found inside the flame envelope. The overall flame shape is observed to change from symmetric (varicose) to asymmetric (sinuous) mode with increasing turbulence intensity due to the reduction of the bulk density ratio between the burnt and unburnt regions. The turbulent flame speed and flame front statistics – curvature, flame surface density, brush thickness, strain rate and turbulent to laminar flame area ratio have been evaluated to quantify the turbulent burning characteristics. Lean flame blowoff equivalence ratio dependence on fuel type and turbulence conditions is also discussed in view of the laser-based measurements. The experimental results from this canonical flame configuration are being used for validation of LES simulations.

B. Roy Chowdhury received his B.S. degree from Jadavpur University in 2012 and is currently a doctoral student in the Mechanical Engineering Department at the University of Connecticut.

B. M. Cetegen received his B.S. (1978) in ME and Physics summa cum laude from Bosphorous University (formerly Roberts College) in Istanbul Turkey followed by M.S. (1979) in ME from UC Berkeley and Ph.D. (1982) in ME from Caltech. He joined the faculty of University of Connecticut in 1987 where he is currently United Technologies Chair Professor.
Instantaneous images of CH$_2$O PLIF, OH PLIF and heat release region overlaid on the vorticity contours / velocity field for high turbulence condition (30 to 31%) corresponding to mean velocity of 10 m/s showing the different characteristics (a) Flamelet merging (b) Occurrence of shear layer extinction (c) Pocket formation (d) Flame fragmentation and (e) Asymmetric flame structure.
Biography

B. M. Cetegen received his B.S. in ME and Physics *summa cum laude* from Bosphorous University (formerly Roberts College) in Istanbul Turkey followed by M.S. in ME from UC Berkeley and Ph.D. in ME from Caltech. After working five years at Energy and Environmental Research Corporation (EERC) as a research engineer and group leader, he became a postdoctoral research fellow at UC Irvine working with Prof. William A. Sirignano. He joined the faculty of University of Connecticut in 1987 where he is currently United Technologies Chair Professor. He has spent sabbatical leaves at Yale University and Ecole Centrale Paris. He has published over 200 research papers in a range of topics including turbulent combustion, detonations and rotating detonations, combustion and plasma synthesis of ceramic materials and coatings, buoyant flames and buoyancy induced instabilities, shock-induced and vortical mixing enhancement, and optical diagnostics of PEM fuel cells. He is a member of the Combustion Institute, a fellow of ASME and an elected member of the Connecticut Academy of Science and Engineering (CASE). He was the chair of the Executive Board of Combustion Institute Eastern States Section (2009-2011) and also served as its treasurer (1999-2007). He served as the department head of Mechanical Engineering from 2006 to 2015. He is the Vice President and President-elect of the Connecticut Academy of Science and Engineering.
Oil Refining in a CO₂ Constrained World: Implications for Transport Fuels Policymaking

Amir F.N. Abdul-Manan, Abdullah Arfaj, Hassan Babiker
Fuel Technology R&D Division, Saudi Aramco Research & Development Center, Dhahran, Saudi Arabia

Diesel compression ignition engines are known to be more efficient, and therefore less CO₂ intensive, than their gasoline spark-ignition engine counterpart. From a fuels’ refining perspective, gasoline would end up having a larger carbon intensity than diesel given that it is composed of streams that have gone through energy intensive processes within the refinery. This is consistently reflected by many LCA studies to date, some of which underpin regulatory measures that favor dieselization.

But, on the contrary, here we show that in a world that internalizes the cost of CO₂ emissions, refineries would favor gasoline over diesel production. A key contributing factor is the refinery hydrogen balance. The shift toward more gasoline allows for the co-production of hydrogen from the reforming unit, and therefore reduces the need for on purpose hydrogen production via steam methane reforming of natural gas, which is more CO₂ intensive. The typical LCA practice of modeling a snapshot of refinery operation today, also known as attributional LCA, is less useful for understanding the consequences of policy actions. The approach that we have taken in this study is effectively a consequential LCA method, which provides better insights to guide policymaking.

This study highlights that the global shift toward transport dieselization can lead to greater refinery CO₂ emissions. But on the other hand, because diesel compression ignition engines are inherently more efficient than a gasoline spark-ignition engine, transport dieselization can help reduce the impact of the transport sector on global greenhouse gas emissions. Here we conclude that an optimum fuel and engine combination is the use of a gasoline-like fuel in an efficient compression ignition engine. It is important that future developments in fuels and engines are integrated to enable a greater overall reduction in transport emissions from Well-to-Wheels.
Oil Heavy Residues Oxy-combustion Demonstration

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Saudi Aramco is conducting pioneering research in energy efficiency and carbon capture, utilization and storage, to help reduce the carbon intensity of its facilities and the utility sector; one possible abatement measure would be the combustion of low value feedstocks and capturing CO₂.

Heavy feedstocks, like oil heavy residues, are most often blended with light ends (i.e., diesel) to enable their transport and qualification as fuel suitable for power plants and utility boiler applications.

Oxy-combustion technology has the potential to combust directly oil heavy residues, by using oxygen instead of air to burn the fuel, which would yield a better combustibility, higher efficiency, and lower emissions, while producing a highly concentrated CO₂ stream that can be easily processed.

Saudi Aramco has conducted with GE a first of a kind testing campaign on a 15 MW thermal industrial scale test pilot facility, firing oil heavy residues, in a step to develop and demonstrate the technology at a significant scale.

The talk would provide insights on the 15 MW testing facility, the testing campaign, and the major findings. It was possible to burn directly the oil heavy residues, with significant improvement in combustion stability, compared to air fired combustion, and reduced carbon loss while reducing significantly nitrogen oxide emissions.
Environmental Impact of Manufacturing Emissions: Taking Cement Industry as a Case

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We are living in a world facing serious interrelated environmental problems, including climate change, pervasive pollution, reduction in biodiversity, and looming supply constraint for a number of key natural resources. Individually, and especially in combination, these issues pose serious challenges to sustainable development. Our aim is to research on global environmental issues and emerging solutions by understanding of environmental science and related policies to increase understanding of the issues involved in tackling the environment and their ability to generate meaningful solutions. The cement industry is generally considered responsible for upwards of 5% of anthropogenic greenhouse gas emissions. This is a result of the high energy intensity of the process, significant CO₂ release from the raw materials used, and large global consumption. It is also a high growth sector as emerging economies develop their infrastructure.

This paper aims to study a carbon dioxide emissions from the cement under the influence of wind conditions. These effects are investigated by Computational Fluid Dynamics (CFD) code used a Large Eddy Simulation (LES) method to study pollution spread in vicinity of manufacturing. The predicted concentration of CO₂ used as the safety criterion provide the useful information about a pollution amount resulted under variant environmental and structural conditions. A detailed look at results is beyond the scope of analysis to determine optimal CO₂ emission.
Process for On-Board CO$_2$ Capture using Hollow Fiber Membrane Contactors

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This work focuses on designing a process for capturing CO$_2$ on-board in transportation vehicles using hollow fiber membrane contactors. In the proposed process, a chemical solvent is used to capture CO$_2$ from the exhaust gas in the contactor, and then the CO$_2$ is released in a stripper, followed by compression in a 3-stage compressor to be finally stored in a tank. The energy required for running the system will come from the waste heat in the exhaust. The work includes process simulation in Hysys and modeling using Excel (for modeling and designing the contactor). The phenomena considered in the modeling are the mass transfer across the membrane, and the reaction between the CO$_2$ and the solvent in the liquid side of the contactor due to their limiting effects on the overall process. Finally, fitting the system in a vehicle chassis will be highlighted as well.

Modeling and simulations results show the following. First, recovered waste heat is enough to support the energy required for capturing up to 50% of the CO$_2$ in the exhaust gas at certain conditions with a specific solvent thus minimizing the extra energy required to run the system. Second, using membrane contactors for capture increases the absorption efficiency by increasing the surface to volume ratio and by acting as a barrier to reduce solvent losses as opposed to the conventional absorption column. Third, due to the higher efficiency of the system compared to the conventional absorption column, the space required is minimized and can fit in any vehicle of an average size.

In conclusion, the system has the potential to reduce CO$_2$ emissions to unprecedented levels that exceeds the policymakers’ expectations as well as providing automakers and stakeholders a short term solution. However further improvement in solvent capacity, membrane & process design can optimize CO$_2$ reduction system. The recovered CO$_2$ can then be further treated at a centralized location for conversion to useful chemicals or sequestered.
On-board Separation for Octane-on-Demand

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Advanced engine-fuel technologies will play a central role in achieving future greenhouse gas emissions targets for light-duty vehicles. One such technology platform is the Octane-on-Demand concept. This concept makes use of an oil-derived fuel at low and intermediate loads where the octane requirement of the engine is comparatively low, while a second high octane fuel is introduced at higher loads to suppress knock. Previous efforts have focused on enabling the Octane-on-Demand concept through the use of two tanks and two fuels with different anti-knock quality. In this work, volatility-based flash distillation is instead used to separate a market gasoline (RON 91) into high and low octane fuels onboard the vehicle. Experimental fuel consumption maps are used to evaluate different drive cycles, fuel economy and greenhouse emissions for a D-segment vehicle equipped with two alternative powertrains. The results show improvements in both fuel economy and greenhouse gas emissions with respect to the conventional vehicle that uses the market gasoline as a single fuel. This study points towards further investigations on Octane-on-Demand as a concept for future spark-ignition engines.
Economic Analysis of High Octane Fuel Implementations

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To establish a new technology in the market, an economic feasibility assessment is a must along with technical feasibility assessment. As a part of Octane on Demand initiative, an economic analysis was conducted to probe the feasibility and reliability of implementing high octane gasoline using different approaches. These alternative scenarios include onboard a vehicle, within a gas station, and in a refinery.

First, onboard separation is a system that separates market gasoline into low and high octane streams onboard a vehicle. Then, the separated streams can be used as a feedstock for the Octane on Demand engine’s concept. Volatility-based distillation was used as a separation technique in the present study. Second, separation in a gas station where gasoline can be separated onsite into high and low octane fuels via a flash distillation or a membrane. Finally, the high octane fuel is produced by gasoline upgrading in a refinery.

This work was completed by designing a module that calculated the capital and operation costs, as well as the benefits, net present value (NPV) and payback period, for the end users and retailers. An analysis of the model sensitivity was conducted. Finally, other factors such as consumer and manufacturer acceptance, regulations, and system complexity were considered. This analysis demonstrated that onboard separation was the most convenient option among the alternatives. This work will subsequently be integrated to support the Octane on Demand engine optimization efforts which target the efficiency and performance enhancement, as well as CO₂ emissions reduction.
Particulate Matter Characterization of Low Cetane Fueled Premixed Compression Ignition PCI Combustion

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A light duty multi-cylinder CI engine running on Premixed Compression Ignition PCI combustion was utilized to mainly investigate the effect of low cetane fuels, including dieseline and naphtha on the particle size-number distributions and chemical characterization of Particulate Matter PM. Different fuel-injection strategies were investigated in a wide engine operating load range from 1.50 to 12 bar BMEP. The introduction of hot Exhaust Gas Recirculation EGR with low injection pressure (as low as 150 bar) for low cetane fueled PCI, significantly reduced the total particle number concentration by about 99% with particles mean diameter \sim 10 \text{ nm} compared to diesel-CI baseline while maintaining NOx below \( (0.27 \text{ g/kw}) \) at low and medium loads. Moreover, the hot EGR reduced the volatile/semi volatile compounds (e.g. PAHs, alkanes, cycloalkanes) in PM of low cetane fuels with respect to the diesel-CI baseline. The utilization of hot EGR could be considered as a "win-win" strategy to enhance combustion process and reduce PM.
Investigation of the Influence of Aromatic on Particulate Emissions during the combustion transition from HCCI, via PPC to CI mode

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The objective of this study is to investigate the effect of aromatic on combustion stratification and nanoparticulate emissions. Experiments are performed in an optical diesel engine at a speed of 1200 rpm for TPRF0, TPRF20 and TPRF40. TPRF mixtures are prepared in such a way that the RON of all test blends are same RON = 60. Single injection strategy with a fuel injection pressure of 800 bar is adopted for all test fuels. Start of injection (SOI) is changed from early to late fuel injection timings, representing various modes of combustion via HCCI, PPC and CI. High-speed video of the in-cylinder combustion process is captured and one-dimensional stratification analysis is performed from the intensity of images. Particle size, distribution and concentration are measured and linked with the in-cylinder combustion images. Results show that combustion advance from CI to PPC and then attains a constant value in HCCI mode. High-speed movies using a color camera showed that more signal in red and green channel is found with high sooting fuels. Soot is increased when adding toluene to a primary reference fuel. The soot mass concentration is higher for late injection timings due to reduced premixing. In PPC and HCCI region, the soot mass concentration was significantly reduced as premixing is improved due to longer ignition delay. There was a link between soot emission (PM) and the combustion stratification, both peaked at SOI= 15 bTDC. The particle number is lower for the late injection and becomes higher as the injection timing advanced to PPC and HCCI mode. While the soot particles are almost nuclear model with the size range of 5nm~17nm and as combustion transit from CI via PPC to HCCI, the particle size becomes larger.
Parametric Optimization of Thermoelectric Generator System Used Exhaust Waste Heat Recovery

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Due to the exponential increase of the global energy consumption, it can be seen that the research potential focuses on technologies that assist to improve the power generation efficiencies especially the one that produced from heat engines. About 40% of the energy produced from combustion systems is discharged to the environment as a form of waste heat through the exhaust system. One way to improve the heat engine efficiency is by using thermoelectric power generator in order to recover the wasted heat. The past few decades show that there are numerous studies on thermoelectric materials in order to improve the thermoelectric figure of merit and eventually the thermoelectric module efficiency. This efficiency is limited by the Carnot efficiency. However, on the system-level, the efficiency of thermoelectric generator system (used to capture exhaust wasted heat) is significantly lower than the module efficiency. Typical thermoelectric generator system consists of thermoelectric module, two heat exchangers, and electrical load. These parameters needs to be optimized (some of them simultaneously) in order to maximize the generated power.

The current work focuses on finding the optimum electrical load resistance of thermoelectric generator system. The optimum load resistance and optimum geometric ratio of a thermoelectric module can obtained simultaneously by using an analytical method that uses the dimensional analysis technique which can be found in the literature. Theses optimum parameters are designed to provide the maximum possible output power of a thermoelectric module attached to two heat sinks. Subsequently, an experiment has been conducted in order to validate the accuracy of the analytical model where a good agreement was observed. Moreover, by using the maximum parameters of the thermoelectric module that are provided by manufacturer, the effective thermoelectric material properties can be obtained; these properties play a big rule to reduce the errors associated with contact resistances and Thomson effect. Moreover, generalized charts were presented in this study which can help designers to determine the optimum load resistance and thermoelectric geometric ratio for the maximum output power.
A minimalist and Functional Group Approach towards Gasoline Surrogate Fuel Formulation

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We present a methodology for surrogate fuel formulation by matching target fuel functional groups, while minimizing the number of surrogate species. Five key functional groups, namely, paraffinic CH₃, paraffinic CH₂, paraffinic CH, naphthenic CH-CH₂ and aromatic C-CH were chosen. Surrogates were developed for six FACE (Fuels for Advanced Combustion Engines) gasoline fuels namely FACE A, C, F, G, I and J. The five functional groups present in the fuels were qualitatively and quantitatively identified using high resolution 1H Nuclear Magnetic Resonance (NMR) spectroscopy. An additional attempt was carried out to minimize the number of surrogate species (maximum 2), so as to reduce the size of surrogate fuel chemical kinetic reaction mechanisms. This would help to reduce the computational expenses and facilitate the simulation of practical devices. The developed surrogates were experimentally validated using ignition delay times (IDT) determined using an ignition quality tester (IQT) as specified by the standard ASTM D6890 methodology and rapid compression machine (RCM) experiments. Research octane number (RON), motor octane number (MON) and derived cetane number (DCN) of the formulated surrogates were also determined and compared with those of the target gasoline fuels. The results showed that the developed surrogates were able to reproduce the ignition characteristics of the target gasoline fuels. This methodology could also be extended to formulate surrogates for other fuels.

Keywords: surrogate; gasoline; functional group; 1H NMR spectroscopy; ignition quality tester (IQT); Rapid compression machine (RCM).
SuperButol™ Technology: New Superior Oxygenate as Gasoline Blendstock

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Driven by the opportunity to develop technologies to valorize low value streams and towards capturing refinery-petrochemical integration benefits, researchers at Saudi Aramco’s R&DC developed SuperButol™ technology, which is a distinctive one-step process to convert mixture of butenes into mixed butanols and iso-octane liquid (SuperButol™) without the need for separation of the isomers. This product has been demonstrated to be a superior gasoline blending oxygenate component that enhances gasoline properties. The SuperButol™ technology can therefore be positioned to play an important role in the fossil-fuel based cleaner burning oxygenate arena by contributing to Saudi Aramco’s Clean Fuels initiative. The technology has been successfully demonstrated using an Integrated Pilot Plant and produced 2.5 tons of on-spec product at 60 kg/day capacity. The product, a mixture of 2-Butanol, tert-Butanol and Di-isobutene, has a high octane rating (RON of 106.7 and MON of 94) with lower Reid Vapor pressure (RVP = 1.6 psi) and is a proposed additive to conventional petroleum-derived gasoline fuels to improve octane performance. It has also been tested for material compatibility, corrosion and fuel properties with no apparent impact on engine components and storage infrastructure. A comprehensive Process Design Package has been developed and is in the process of getting deployed at a commercial scale (80-340KTA).
Biodiesel Production from Karaya Oil via Transesterification using Methanol

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The investigation of unknown and non-edible vegetable oil called karaya thought of to be a promising economic exploration in the field of biodiesel in the semi-arid regions. This research will aim to describe the process of transferring karaya oil into biodiesel using the method of transesterification hopefully under supercritical conditions. The methyl ester of karaya oil might have several outstanding advantages among other new-renewable and clean engine fuel alternatives. The factors affecting the production of biodiesel during the transesterification reaction are all under investigation, such as molar ratio (alcohol:oil) and reaction temperature. It’s grasped from literature that the karaya oil extracted from a tree called Sterculia Striata, this tree produce a fruit called foetida which has seeds that contain up to 41% in oil. Up to 50% of the fatty acid contain cyclopropenoid ring. Moreover, it was observed that the cyclopropenoid ring remains after transesterification and is decomposed during pyrolysis. Although, verification of this still under process by using Gas Chromatography to test the yield physical/chemical properties. Prior that, a simulation will take place to try to optimize the system before its being built.

Some studies in literature showed that oil extracted from Sterculia Striata tree meets biodiesel standards in acceptable range. Therefore, this study will aim to prove the global advantages of using karaya oil as a substitution over conventional diesel as well as newly invested other alternatives.
Effect of Ethanol Addition on Low Temperature Chemistry of PRF Mixture

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Ethanol blended in Primary reference fuels have earlier shown a non-linear trend in octane improvement tendency. However, little explanation has been given on the underlying phenomenon that results in this behavior. In this study we aim to study the octane improvement tendency of ethanol using HCCI engine experiments. Knock is merely autoignition of the end-gas as first shown in Sir Ricardo, hence HCCI engine, which relies on autoignition tendency of the fuels can give better insight on the knocking tendency also. In this regard, experiments performed in a single cylinder CFR engine with varying concentration of

Ethanol in PRF70 mixtures show Low temperature chemistry (LTC) suppression with ethanol addition. It is also seen that LTC phase retards with increasing ethanol concentration, which leads to increased temperature before the onset of high temperature chemistry. The net autoignition tendency of the fuel mixture is a composite effect of the magnitude and phasing of the LTC, which are both effected with increasing ethanol concentration. This work also, in effect, explains the non-linearity in octane improvement tendency showcased by ethanol gasoline blends by several researchers over the years.
Ion Chemistry Investigation in Premixed Rich to Near Soot Methane Flame

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Applications of electric field or plasma on flames show great influences on enhancing combustion behavior, including emission suppression, flame stability extension, spark ignition promotion and efficiency improvement. Ion chemistry plays an important role in plasma/ electric field enhanced combustion, although ions produced by chemi-ionization reactions in flames have low mole fraction, varying from 10^{-7} to 10^{-9}. To better understand the enhancement on flames from electric field, ion chemistry need to be built and developed. In our previous work, ion profiles in low pressure premixed methane flame under lean to slightly rich region were measured experimentally, and compared with ion chemistry model simulation. H3O+ was the most dominant ions over the entire flame zone, and other ions like C2H3O+, C3H3+ in the flame zone were also observed. In this work, further investigation was conducted on rich to near soot zone. Three low pressure flames (p=60 torr), with varying equivalence ratios from 1.5, 1.8 and 2.0 was experimentally investigated with quadrupole Molecular Beam Mass Spectrometry. Besides that, ion profiles were also measured under higher pressure flame (p=90torr) to investigate pressure effect and complete ion profiles in entire flame zone. Neutrals in the same flames were measured using Synchrotron Vacuum Ultra Violet Time Of Flight Molecular Beam Mass Spectrometry at Advanced Light Source. Experimentally, C3H3+ was found to be the most dominant ions over the entire flame zone, which is different from lean and stoichiometry flames, suggesting different chemistry exist. An updated ion chemistry model based on ArmacoMech 2.0 neutral model was proposed, and used to compare with experimental data. Rate of production analysis was performed later to assess reaction pathways of different ions. This work can provide experimental data of ion profiles in premixed flames, and used to develop ion chemistry model in the future, which could be used for guidance of electric field application on internal combustion engines.
Simulations of fluidized Bed Reactors for Chemical Looping Combustion: Effect of Wall and Particle Interactions

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Chemical looping combustion (CLC) is an innovative concept and attractive option to capture carbon dioxide (CO$_2$) with a significantly lower energy penalty than other carbon capture technologies. It generally consists of a fuel reactor (FR) and an air reactor (AR) operating in a bubbling/circulating fluidized bed regimes. In the current study, a conceptual reactor configuration has been studied in which the FR is an annular fluidized bed (AFB) reactor and the (AR) is in circulating fluidized bed regime and is placed concentric to the AFB. This is to utilize the heat transfer through the walls of the AR. In this type of reactor, the solid interaction with the walls is higher than in the cylindrical reactor due to the presence of inner and outer walls. A major advantage of such a reactor is better mixing of the reactor contents (gas/solids) which would enhance the reaction rate. Mixing depends greatly on the solid velocities, bubble formation etc. which in turn are influenced by the wall boundary conditions, particle-particle and particle wall interactions.

Specularity, particle-particle and particle wall restitution coefficients significantly influence the solid flow pattern in a bubbling flow regime. In particular, the restitution coefficients affects the uniformity of the bed which affects the reaction rate. Besides, the fluid dynamic properties of the reactive flow behaves entirely different from that of the cold flow. Therefore, it is important to study the effect of these coefficients on the chemical process performance in addition to the hydrodynamics of the cold flow. A study of the reactor hydrodynamics and the chemical process will serve the purpose of optimizing the performance of the reactor. In the current study, an annular methane-fuelled CLC reactor which operates in the bubbling flow regime has been simulated. The simulations are performed by using a two-fluid model, employing the conservation of mass and momentum for both the fluid and solids (iron oxide particles) with chemical reactions in an open source code (MFiX) developed by National Energy Technology Lab. The results indicate that a circumferential core annulus structure is obtained in the reactor which is different from that of a cylindrical reactor. The effect of the wall boundary conditions and particle interactions on the hydrodynamics of the reactor is significant which can also be seen on the chemical performance of the reactor. The results obtained will help in optimizing the performance of the reactor under study.
The Optimization of Paper Discoloration via Carbonization using a CO\textsubscript{2} Laser for Inkless Black-and-White Printing

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Printing ink is considered the most expensive liquid among consumer goods after perfumes. Ink also has environmental drawbacks starting from its production, transportation, and disposal. In fact, ink makes recycling paper more challenging as ink adds a de-inking step that is energy intensive and uses corrosive chemicals. This research proposes a new technique that revolutionizes black and white printing, and eliminates black ink in printers completely (Alhashem et al., 2015).

Using a 75-watt carbon dioxide (CO\textsubscript{2}) laser, emitting a 10.6 \textmu m wavelength beam for heating, we are discoloring the surface of the paper by converting paper’s cellulosic structure into carbon. This conversion is essentially a combustion reaction. Solid fuel burns in three stages: drying, devolatilization (pyrolysis, distillation phase), and lastly, the char (charcoal) combustion. We augment these stages with heat from the CO\textsubscript{2} laser. Moving the laser rapidly above the paper surface arrests the reaction at the second stage, after the formation of blackened char. A special software is used to control the movement speed of the laser, laser power, and distance from the paper. The optimization process aims at maximizing the darkness of the discoloration while maintaining the quality of the paper. For characterization and quantifying discoloration, a UV-Vis spectrometer with an integrating sphere is used to measure the absorption of light in the discolored regions.

References:
Ignition Delay Time Correlation of Fuel Blends based on Livengood-Wu Description

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In this work, we report universal methodology for ignition delay time correlation of multicomponent fuel mixtures in a wide temperature, pressure, equivalence ratio region. N-heptane, iso-octane, toluene and ethanol are investigated in this study because of their relevance to gasoline fuel surrogates formulation. The proposed methodology combines benefits from the Livengood-Wu integral, the cool flame characteristics and the Arrhenius behavior of the high temperature ignition delay time to get a simple and comprehensive way to correlate the ignition delay times of pure components and mixtures of them. The ignition delay times (IDT) of fuel mixtures normally have complex dependences on temperature, pressure, equivalence ratio and composition of the fuel blends. Here, the Livengood-Wu description of ignition phenomena is presented and it is proved that the Livengood-Wu integral is valid without imposing the zeroth order kinetic assumption which is usually applied. The Livengood-Wu integral is applied to relate the NTC region to the cool flame phenomena. The Livengood-Wu integral is also extended to get to a relation between the IDT of single component fuels and the IDT of mixtures. The calculated IDT of n-heptane, iso-octane, toluene, ethanol and mixtures of them using the proposed methodology are in excellent agreement with the simulated ones using a detailed chemical kinetic scheme (FACE gasoline surrogate mechanism of Mani et al. 2016 [1]). Finally, homogeneous charge compression ignition (HCCI) simulations are performed using a detailed chemistry and the results are compared with the predictions using the developed correlation. Very good agreements are observed where most of the deviations in the combustion phasing are within 1 crank angle degree.

Estimating Fuel Octane Numbers from Homogeneous Gas-Phase Ignition Delay Times

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Fuel octane numbers are directly related to the autoignition properties of fuel/air mixtures in spark ignition engines. This work presents a methodology to estimate the research and the motor octane numbers (RON and MON) from ignition delay time (IDT) data calculated at various pressures and temperatures. The hypothesis under investigation is that at specific conditions of pressure and temperature (i.e., RON-like and MON-like conditions), fuels with IDT identical to that of a primary reference fuel (PRF) have the same octane rating. To test this hypothesis, homogeneous gas-phase IDTs with a detailed gasoline surrogate chemical kinetic model have been calculated at various temperatures and pressures. From this dataset, temperatures that best represent RON and MON have been correlated at a specified pressure. Correlations for pressures in the range of 10-50 bar were obtained. The proposed correlations were validated with toluene reference fuels (TRF), toluene primary reference fuels (TPRF), ethanol reference fuels (ERF), PRFs and TPRFs with ethanol, and multi-component gasoline surrogate mixtures. The predicted RON and MON showed satisfactory accuracy against measurements obtained by the standard ASTM methods and blending rules. The correlations were also validated against an extensive set of experimental IDT data obtained from literature with a high degree of accuracy in RON/MON prediction.
Long Term Technology Outlook for Light Duty Vehicles

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Many technology-based changes are set to impact the light duty vehicle (LDV) market over the coming years. These include the advent of cheaper Li-Ion batteries, more sophisticated internal combustion engine technology, vehicle design improvements, and the whole gamut of behavior changes associated with the generic title “mobility”. This study by Saudi Aramco’s Technology Strategy and Planning Department seeks to understand the techno-economic impact of these changes by modelling a mass market mid-sized car (in this case a Malibu) with seven different drivetrains, using sufficient available technology to meet CAFÉ regulations over time, and seeing how these compare. This study is intended to be unbiased, seeking only to interpret available data from a “bottom-up” perspective. It indicates the evolution of viable electric vehicles, how the market is likely to evolve, and the challenges to be faced by OEM's.
Physical Properties Effects of Low Octane Gasoline on the Combustion and Emissions of GCI Engines

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One of the attractive alternatives to traditional spark ignition engines is the gasoline compression ignition (GCI) engine technology. Fuels with octane numbers lower than those of market gasolines have been identified as a viable option for GCI engine applications. Their longer ignition delay time characteristics compared to diesel fuel and their similar volatility features compared to gasoline fuels make them interesting to be explored. This study focuses on investigating the effects of the fuel's physical properties on GCI engines performance. The fuel's physical properties are altered separately to isolate the effect of each property and investigate its impact on the engine combustion and emissions at medium load conditions. The base fuel is a mix of refinery streams with a RON of 75 and physical properties in the gasoline range. A primary reference fuel (PRF), a mixture of n-heptane and iso-octane, chemical surrogate utilized in the engine computational fluid dynamics (CFD) simulations. The physical properties of the base fuel and its variants were imposed on the PRF surrogate to mimic the physiochemical properties of the GCI fuel. The examined physical properties were viscosity, density, heat of vaporization, surface tension, heat of capacity, vapor pressure and thermal conductivity.
CFD Study of Rate Shaping With Multiple Fuel Injectors to Reach Higher Efficiency

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Higher efficiency is something much needed for future combustion engines and is therefore of big relevance. One way to achieve this is through a more ideal heat release in the engine cycle, such as isochoric combined with isobaric combustion. There are many previous studies regarding this matter and one common way to achieve more optimal heat release timing is by using boot shaped injection, which controls the injection by releasing more fuel later in the cycle. However there are newer studies showing that the heat release can be controlled even better when using three different injectors in a CI engine.

The Computational Fluid Dynamics (CFD) study here concerns this multiple fuel injector strategy. Different injection pulse strategies are implemented to achieve the controlling of the combustion heat release. Simulations were carried out using the software Converge on a Volvo D13 cylinder geometry with three standard injectors and changed compression ratio.

Results from the simulations showed that it is indeed possible to control the heat release better with three injectors compared to one injector. Using the CFD enables a more swift and flexible way of changing certain parameters in order to perform future testing and experiments which is valuable when doing parameter sweeps.
Ethanol-Gasoline Fuel Blend Combustion Study in Si Engine

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In this study, the effect of ethanol in gasoline combustion engine has been investigated and optimized from emission and performance point. At the first level, the engine performance for pure gasoline fuel; then a mixture of ethanol and gasoline was used in which the amount of ethanol varies from 1% to 20%. The engine speed was chosen 2000 rpm and single fuel gasoline was compared to ethanol-gasoline fuel blend. Engine performance was validated by different results and shown in figure 1.

From the performance and emission value points it was obvious that 8% ethanol-gasoline blend is the desirable amount. It is clear that from performance and CO point, there is a good agreement between the results and literature researches. Figure 2 shows the change of CO and CO2 as a function of crank angle. In general, the results showed similar trends except the ones using SRM-detailed chemistry. The accuracy of the results were tested by comparing to each other literature data, especially when it is considered that SRM detailed chemistry results are in good agreement with experimental out comes in terms of the available data.
CFD-Guided Gasoline Compression Ignition Engine Calibration

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One of the attractive alternatives to traditional spark ignition engines is the gasoline compression ignition (GCI) engine technology. Fuels with octane numbers lower than those of market gasolines have been identified as a viable option for GCI engine applications. Their longer ignition delay time characteristics compared to diesel fuel and their similar volatility features compared to gasoline fuels make them interesting to be explored. In this study, we have numerically investigated the effect of different injection timings at part-load conditions using a research octane number (RON) 75 fuel in gasoline compression ignition single cylinder engine. Full cycle GCI computational fluid dynamics (CFD) engine simulations have been successfully performed while changing the start of injection (SOI) timing from -60o to -10o CAD aTDC at 5 bar indicated mean effective pressure (IMEP). The effect of SOI on mixing, combustion phasing and engine-out emissions is investigated using detailed equivalence ratio-temperature maps. Also, the effects of different rates of exhaust gas recirculation (EGR) on the combustion and emissions characteristics are investigated. Rebreathing valves profiles along with double injection strategies are also examined in the current study. Fuel consumption, soot, nitric oxides (NOx), hydrocarbon (HC) emissions and combustion phasing (CA50) are the targeted parameters throughout this study.
Experimental studies for the Thermo-physiochemical properties of BioDiesel and its Surrogates and the performance of such fuels in a Compression Ignition Engine

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Biodiesel from vegetable oil source is used to produce surrogate fuels mixing it with red diesel. The fundamental thermochemical properties were measured using standard STMD methods and compared with other experimental data available. Some of the main properties such as density and viscosity showed a linear variation with the percentage of Biodiesel in the surrogate while others such as cetane number is high for surrogates with larger percentage of Biodiesel.

Samples of the surrogate, mainly B25, B50 and B75, where the figure stand for the percentage of Biodiesel, in the mixture were tested in a compression ignition engine. The objective is to study the thermal and emission performance of such fuels and attempt to explain the difference reverting to the thermochemical analysis done for the fuels.

The engine data has shown that the surrogate fuel B75 produces both best thermal performance and less emission compared to Biodiesel, Diesel and the other two surrogates. Most likely the reason behind this is due to the chemical composition (microstructure) of the fuel. The spectra for B75 produced using gas analyser has shown that B75 has a complex composition compared to other fuel with a few hydrocarbon and oxygenated groups dominating the elemental content of the fuel. It is thought that this composition offered B75 the superiority in terms of efficient burning under the current combustion infrastructure (CIE), leading to both better energy release and less emissions.

Figure 1: Cetane number

Figure 2: Spectra: D100, B100, B20, B40, B60 and B80

Figure 3: CIE thermal efficiency
Physical and Chemical Effects of Low Octane Gasoline Fuels on Compression Ignition Combustion

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Gasoline compression ignition (GCI) engines running on low octave gasoline fuels are considered an attractive alternative to traditional spark ignition engines. In this study, three fuels with different chemical and physical characteristics have been investigated in single cylinder engine running in GCI combustion mode at part-load conditions both experimentally and numerically. The studied fuels are: Saudi Aramco light naphtha (SALN) (Research octane number (RON) = 62 and final boiling point (FBP) = 91°C), Haltermann straight run naphtha (HSRN) (RON = 60 and FBP = 140°C) and a primary reference fuel (PRF65) (RON = 65 and FBP = 99°C). Injection sweeps, where the start of injection (SOI) is changed between -60 and -11 CAD aTDC, have been performed for the three fuels. Full cycle computational fluid dynamics (CFD) simulations were executed using PRFs as chemical surrogates for the naphtha fuels. Physical surrogates based on the evaporation characteristics of the naphtha streams have been developed and their properties have been implemented in the engine simulations. It was found that the three fuels have similar combustion phasings and emissions at the conditions tested in this work with minor differences at SOI earlier than -30 CAD aTDC. These trends were successfully reproduced by the CFD calculations. The chemical and physical effects were further investigated numerically. It was found that the physical characteristics of the fuel significantly affect the combustion for injections earlier than -30 CAD aTDC because of the low evaporation rates of the fuel because of the higher boiling temperature of the fuel and the colder in-cylinder air during injection.
Shift in Combustion Homogeneity from CI combustion towards HCCI

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Low temperature combustion (LTC) concepts are widely studied for simultaneous reduction of NOX and soot emissions. Amongst several combustion concepts, partially premixed combustion (PPC) has better control over combustion and it reduces the engine out emissions without compromise in efficiency. This study explains the shift in combustion homogeneity from compression ignition (CI) towards homogeneous charge compression ignition (HCCI) via PPC by advancing the start of injection (SOI).

PRF60 is tested in an optical diesel engine at low speed (1200 rpm) and low load condition (IMEP = 2 to 3 bar). The baseline data is recorded for diesel at an absolute intake pressure of 1.55 bar and intake air temperature of 35°C. However, PRF60 required an intake air temperature of 90°C to match the combustion phasing of diesel. The combustion phasing is separated from SOI during HCCI condition, while intake air temperature and SOI controlled the combustion phasing in PPC mode. With dilution (18% oxygen in the intake), combustion phasing is retarded and intake air temperature is increased to compensate this. With the advancement in SOI, premixing is enhanced and combustion turns homogenous at very early injections. At late injection timings, natural luminosity of the combustion images is higher, while it decreases as SOI is advanced. The combustion images are correlated with in-cylinder pressure and rate of heat release to attain better insights on combustion homogeneity. Stratification analysis, based on intensity of images, shows that diesel combustion is more stratified when compared to PRF60. When compared to diesel, soot flames are less evident in PRF60 and weak luminous flames are an indication of premixed combustion.
Effect of fuel octane rating on combustion stratification in an optical diesel engine

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Fuel octane rating is important in partially premixed combustion as it creates the required ignition delay for premixing. This premixing effect enables simultaneous reduction of NOX and soot emissions. In this study, influence of fuel octane number on combustion stratification during PPC is investigated. For this, fuels with same physical properties but different octane ratings are chosen. Fuels considered in the current study are PRF0, PRF50 and PRF65, which are tested in a direct injection optical diesel engine. Single injection strategy is adopted, while fuel is injected at a pressure of 800 bar for an engine speed of 1200 rpm. Combustion phasing is kept constant for all fuels by varying the intake air temperature. High speed video of the combustion process is recorded through a high speed camera and the images are processed to estimate the level of stratification for all the test fuels with different octane rating.

The experimental study demonstrates that combustion phasing is related to start of injection (SOI) during late injection, while it detaches at early injection for all test fuels. For a constant temperature sweep, combustion starts to destabilize at very early SOI due to lean burning. In this study, the combustion duration is increased with the increase in octane number due to higher intake air temperature. Also, the low temperature reaction (LTR) phase is not evident for PRF0, while PRF50 and PRF65 show a prominent LTR regime. Combustion is premixed for PRF0; the decreased luminosity of combustion images is an evidence to this. The level of stratification is higher for PRF50 and PRF65 when compared to PRF0 due to decreased effect of premixing. Further, the emission results of total hydrocarbon (THC) and carbon monoxide (CO) show a decreased trend with the increase in RON. While the soot concentration is lower for all the test fuels, NOX emission is higher for high RON fuels due to higher intake air temperature.
Ignition Delay Measurements of Straight Run Naphtha

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Most of the energy for transportation is currently obtained from the internal combustion (IC) of liquid fuels which are mainly extracted from crude oil. Refineries must perform elaborate processing of the crude oil to obtain gasoline and diesel. Such processing leads to high CO₂ emissions from the refining process. Crude oil consists of 15 to 30% of naphtha by weight, depending on the source of the crude oil. Naphtha is one of the products of the initial distillation and thus needs less processing (less energy consumption) for its production. As result, the refining process will have lower impact on the environment from CO₂ emission.

In this work, we have performed experimental and modeling work to assess the ignition characteristics of naphtha for its use in gasoline compression ignition (GCI) engines. A global indicator of fuel ignition and reactivity is the “ignition delay time” which is measured in ideal reactors, such as shock tube and rapid compression machine. Here, we measured the ignition delay times of Haltermann straight run naphtha (HSRN) over wide ranges of pressures, temperatures and equivalence ratios.

The naphtha used here has research octane number (RON) of 60 and motor octane number (MON) of 58.3. The ignition delay times of HSRN were measured over the following conditions:
Temperature Range: 620 – 1250 K, Pressures: 20 and 60 bar, Equivalence ratios: 0.5, 1 and 2

To perform computational fluid dynamic (CFD) simulations of complex real fuels, such as naphtha, a simpler surrogate fuel with small number of components must be proposed which matches the properties of the real fuel. In this work, we have compared the ignition of HSRN samples with the predictions of three surrogates: (1) a two-components primary reference fuel (PRF) surrogate comprising of n-heptane and iso-octane, which matches the RON of HSRN, (2) a Three-components toluene primary reference fuel (TPRF) surrogate containing of toluene, n-heptane and iso-octane, which matches the RON and MON of HSRN, (3) a six-components surrogate which matches the RON, MON, H/C ratio and distillation curve of HSRN. We observed that at high and intermediate temperatures (T > 800 K), all PRF, TPRF and multi-component surrogates have good agreement with our experimental
ignition delay data. However, at lower temperatures, multi-components surrogate appears to better emulate the ignition characteristics of naphtha.
Experimental Characterization of a Swirl-Stabilized Premixed Turbulent Burner for the Study of Thermoacoustic Instabilities

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Combustion instabilities are a major issues during the design and operative phase of gas turbines and aero-engines especially if they are working at equivalence ratio lower than one (lean configuration). The coupling between heat release rate from the flame and the acoustic field inside the combustor can generate self-sustained instabilities, called thermoacoustic instabilities, which can deteriorate the combustion process and even lead to structural failure of the entire system. In real combustion systems, the flame is usually stabilized using swirler through the generation of a system of recirculation zones. Typically, the interaction between the acoustic field (acoustic waves) and the flame (heat release rate fluctuations) is analyzed via evaluation of Flame Transfer Function (FTF) that relates velocity oscillations to the heat release rate fluctuations. In this study, the characterization of a swirl-stabilized premixed flame burner for turbulent flame dynamic studies is carried out. The experimental apparatus is composed by a swirl-stabilized burner of 4 kW thermal power, a quartz tube to confine the flame, a hot wire anemometer to measure the velocity and a loudspeaker system for flame transfer function determination. The optical diagnostics comprise a photomultiplier detector to collect CH* chemiluminescence signal and a Particle Image Velocimetry (PIV) system. The tangential and axial velocity fields for cold case are measured by PIV and a swirl number equal to 0.4 is evaluated. The flame transfer functions for 5% and 8% of forcing amplitude for a mixture of methane/air with equivalence ratio of 0.68 are obtained. The evaluated behavior of gain and phase of the flame transfer function are similar to previous studies on this type of flame configuration. All the collected data are used to fully characterize the apparatus and they will be the reference for future experiments at high pressure.

![Graph](image)

Figure: Gain (a) and phase (b) of the flame transfer function for two different levels of excitation.
Steam Reforming of CH$_4$ in a Temperature-Controlled Dielectric Barrier Discharge Reactor

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Due to its advantages of compact, fast response and free from coking etc., plasma technology attracted more attention as a promising technology for upgrading hydrocarbons over recent years. However, the deeper understanding and explanation to plasma reforming processes are still very limited, especially for the non-thermal plasmas. Commonly, plasma chemical processes are determined by the initial plasma-induced chemical and the following thermo-chemical processes. The initial process produce the radicals, ions and excited molecules, which can induce the following thermo-chemical reaction to result the finial target products. In order to investigate the two processes in plasma reforming, we developed a temperature controlled dielectric barrier discharge (TCDBD) reactor, which can individually control the plasma factors and temperature.

By using the TCDBD reactor, dry reforming and partial oxidation of CH$_4$ were studied in our previous work. The study of endothermic dry reforming of CH$_4$ indicates that plasma-induced chemical process govern the conversions of CH$_4$ and CO$_2$, and the thermo-chemical process determines the products selectivities. The test of exothermic partial oxidation of CH$_4$ shows that the plasma-induced and thermo-chemical processes enhanced to each other. In this work, we continuously, study the steam reforming of CH$_4$ in TCDBD reactor. The effects of power, gas composition, pressure and temperature on steam reforming in plasma were tested. The determining factors of the conversions of hydrocarbons and the products selectivities were explored. Electron collision processes in steam reforming were analyzed based on Boltzmann equation for various experimental conditions. The main electron processes and reactive species during steam reforming in TCDBD reactor were studied.
A Computational Study of Ionic Wind Effects on Dynamics of Nonpremixed Counterflow Flames Subjected to DC Electric Fields

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The role of electric fields in improving combustion has been observed since decades. The mechanism of the interaction is generally supposed to be the ionic wind, which is created by the action of the electric field upon the ions naturally produced in flames. The ionic wind changes the flow dynamics in the flame front region and significantly affects the dynamics and structure of the flames. However, the role of the ionic wind needs further investigation in order to provide fundamental understanding of the complex interaction of the electric field and the flame-generated ions and electrons. In this study, numerical simulations were performed to analyze the effects of DC electric fields on the behavior of nonpremixed counterflow flames, with an emphasis on the modification of the velocity field caused by the ionic wind. The distribution of the charged species and electric field was computed based on detailed two-dimensional numerical simulations using approaches similar to previous studies. The equations of Navier-Stokes coupled with transport equations for neutrals and charged species’ mass fractions along with a Poisson equation for the electric potential were solved using the OpenFoam code. The model reproduces tendencies of experimental observations. When the voltage is increased the flame first changes its axial position by moving towards the cathode and then, when saturation of current is reached, any further increase of the bias voltage does not modify the flame behavior anymore. An interpretation of the effect of ionic wind on the propagation and stabilization mechanisms of the flame under a bias voltage was proposed based on an analysis of the current-voltage characteristics.
The Potential and Challenges of Natural Gas as Ground Transportation Fuel in Saudi Arabia

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Natural gas is the most widely used alternative fuel for ground transportation. There are currently more than 22 million of natural gas vehicles with more than 26 thousand refueling stations in 86 countries. The widespread use of NG in ground vehicle is mainly attributed to its easy adaptability to SI and CI engines, low unit price and cleaner exhaust emissions. They are especially used in countries where fuel price relatively high to the public. NGV has proven to reduce urban air quality. NG engines produce 25\% less carbon dioxide than gasoline and 35\% less than diesel, reduce carbon monoxide emissions by 95\% compared to gasoline, hydrocarbons emissions by 80\% and nitrogen oxides' by 30\%. Particulate emissions is virtually eliminated. NG can be used as sole fuel or operate alongside with gasoline and diesel in dual-fuel or bi-fuel engines. But there are technical challenges with NG engines to be solved – high NOx and THC emissions in addition to reduced power and limited driving range. In Saudi Arabia, vehicle numbers and urbanization of population is rapidly developing. More than 80\% of population dwell in cities, resulting in high concentration vehicle exhaust gas polluting the air. The potential of using natural gas as ground transportation fuel in Saudi Arabia is discussed. NGV can mitigate the country’s air pollution challenge especially in urban areas. Vehicle total ownership cost (TOC) can be reduced significantly when combing NG price and reduced maintenance cost. It will diversify the domestic use of abundant NG resources while reduce dependency to gasoline and diesel. Taxis and commercial medium and heavy duty commercial vehicle are clear candidates to take advantage of NG. Implementation of NG as ground transportation fuel are faced by challenges that can be divided to three categories – infrastructure, culture/policy and technical. To be most effective, the NG pipeline network need to be extended to major cities and refueling stations equipped with NG dispenser. The convenience and low price of conventional fuels is the major obstacle to break. There is also a misinformed safety concern having high pressure NG tank on-board vehicle. While at the same time, technical issues with respect to GHC emission of methane from engine misfiring and blow-by must be carefully addressed. If challenges can be addressed sufficiently, Saudi Arabia can benefit significantly from the penetration of natural gas.
Investigation of the Unsteady Effects of Temperature Fluctuation on the Ignition of a Hydrogen-Air Mixture

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The importance of the present work is closely related to the modern engine applications such as homogeneous charge compression ignition (HCCI) or low temperature combustion (LTC) engines in which wall heat losses or the presence of residual gasses may cause the temperature stratification. Then, from Lagrangian point of view, a locally reactive mixture pocket is subject to temporal fluctuations in temperature or concentration during the induction period, and depending on the fluctuating level, the response of the ignition delay time may differ. Thus, accurate interpretations of the ignition response against different types of fluctuation should be delivered to design the engines appropriately.

The present study investigates the unsteady effects of the temperature fluctuation on the ignition of a homogeneous constant pressure hydrogen-air mixture. For this purpose, two sets of initial conditions have been considered such that hydrogen combustion at both chain branching (above crossover temperature) and thermal (below crossover temperature) explosion regimes are investigated. The analysis was conducted by using mathematical tools generated from the Computational Singular Perturbation (CSP) framework, that their validity has been widely tested. In particular, these tools enable the local identification of the most important species and reactions to the ignition delay time.

In overall, the results of a wide range of amplitude and frequency conditions showed that the response of the ignition delay time according to the frequency imposed exhibited an oscillatory decaying trend such that at the infinitely high frequency, the ignition delay time tended to converge to a single value. It was also found that regardless of explosion regimes, once a positive temperature fluctuation was imposed, the ignition delay time was always shorter than that of the unperturbed (reference) case. The results obtained from CSP showed that in that case, the mean characteristic time scale of the system is always smaller than that of the unperturbed case. The reactions that contributed the most to the generation of the characteristic timescale of the system in both cases (oscillating temperature and reference) were identified and their contributions were compared at selected representative points of the process. The analysis revealed that the response of these reactions to the temperature oscillation produces a positive outcome per cycle, from the very beginning of the process. As a result, when a positive temperature fluctuation is imposed, the ignition delay time is decreased.
Experiments on Turbulent Non-Premixed Syngas Flames at Elevated Pressures

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The Turbulent Non-premixed Flames (TNF) Workshop was established twenty years ago to enhance the study of turbulent combustion in a coordinated and collaborative way. Flames that have been selected for inclusion in the workshop are characterized by simple boundary conditions and relatively simple chemistry for the purposes of validation of numerical models. Despite the impressive gains in understanding made by this workshop, there are still very few experimental results from turbulent non-premixed flames (TNFs) at elevated pressures. The high-pressure combustion duct (HPCD) at KAUST was developed specifically to address this concern. In this presentation, results from recent experiments in the HPCD will be presented, with a focus on syngas flames. Nine turbulent syngas (CO/H2/N2) flames were tested at pressures up to 5 atm and with a range of Reynolds numbers from 16000 to 83000. The baseline case (P = 1 atm, Re = 16,700) is part of the TNF library (known as the Sandia/ETH-Zurich chnA flame) and has been studied extensively. Four of the pressurized cases maintain the same Reynolds number as the baseline case and the other four pressurized cases maintain the same bulk jet velocity as the baseline case. All of the flames are momentum-dominated, and direct imaging shows that the flame height is only moderately affected by changes in pressure and Reynolds number. High-speed OH-PLIF images are used to show changes in reaction zone thickness with pressure and increased flame corrugation and localized extinction with increasing Reynolds number.
Chemical Looping Combustion & Calcium Looping for CO₂ & SO₂ Capture from Heavy Fuel Oil Fired Power Plants

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Heavy fuel oil (HFO), the residual heavy fuel fraction obtained from petroleum distillation, is an inexpensive highly sulfated fuel that is fired in many power plants in Saudi Arabia. The integration of carbon capture and sequestration (CCS) at HFO-fired power plants decouples HFO combustion from CO₂ emission, and can therefore ease environmental concerns while tolerating economic incentives to continue to utilize HFO. However, this process is complicated by sulfur dioxide (SO₂) generation during HFO combustion and the many other impurities present in HFO.

Calcium looping (CaL) and chemical looping combustion (CLC) are two emerging CCS technologies that seem promising for local implementation. CaL is a high temperature post-combustion CO₂ separation process that utilizes calcium oxide (CaO) to simultaneously concentrate CO₂ and capture SO₂. CLC is an advanced oxy-combustion technology that makes use of an oxygen carrier (OC) to avoid direct contact between fuel and air during combustion, therefore intrinsically eliminating combustion product gas dilution in air.

The objective of this study is gauging the potential of incorporating CLC, CaL or a combination of CLC & CaL at HFO-fired power plants. Power plants with different configurations were simulated and power cycle analyses and parametric studies were performed on each of these configurations. At select conditions the simulated HFO-fired power plant with integrated CaL is theoretically capable of achieving 95% CO₂ capture efficiency, ~100% SO₂ capture efficiency, and CO₂ compression to 200 bar while maintaining ~89% of reference plant efficiency. The simulated HFO-fired CLC plant is theoretically capable of achieving ~100% CO₂ capture efficiency, ~99% SO₂ capture efficiency, and CO₂ compression to 200 bar while surpassing reference plant efficiency. With respect to energy efficiency penalty, this study indicates that the simulated combined CaL/CLC process is not competitive, while, theoretically, CaL and CLC individually are competitive and promising approaches for CO₂ and SO₂ capture from HFO-fired power plants.

As data is limited, these predictions do not account for the effects of HFO impurities on OC or CaO regenerability. Additionally, the overall feasibility of CLC is unknown since kinetic data on HFO oxidation by OCs is limited. A reactor was designed and constructed to (1) screen OC/HFO reactivity, (2) study CLC and CaL chemical kinetics and (3) explore OC/CaO regenerability at the optimal operating conditions delineated by the parametric study. Progress will be presented.
Simplified schematic diagrams of the HFO-fired power plants with integrated (a) CaL, (b) combined CaL/CLC and (c) CLC.
Ozone Activated Cool Diffusion Flames of Butane Isomers in Counterflow Facility

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Proceeding from the aim to reduce the global pollution emissions caused by the burning of hydrocarbons due to the significant growth in energy demand, more efficient and ultra-low emissions engine concept such as homogenous charge compression ignition engine (HCCI) has been developed. A detailed investigation on the properties of cool flames, governed by low temperature chemistry (LTC), is essential in designing these new types of engines since it is related to some combustion phenomena such as autoignition, knock, and soot. Therefore, the main aim of this work was to build a fundamental counterflow experimental facility for cool flame studies in diffusive system to better understand combustion in LTC engines. This project intended to provide a basic understanding of the low-temperature reactivity of butane isomers under atmospheric pressure condition. This has been achieved by establishing self-sustaining cool flames through novel technique of ozone addition to oxygen stream in non-premixed diffusive counterflow setup. The critical ignition and extinction of cool flames of butane isomers have been investigated under a variety of strain rates. The results revealed that establishment and sustenance of cool diffusion flames are favored at lower strain rate and higher fuel stream temperatures. It has been also observed that ignition and extinction concentrations are directly proportional to the strain rate. The ignition limits of iso-butane cool diffusion flame found to higher than n-butane, reflecting the differences in their reactivities. The effects of ozone concentration on cool flame ignition limits for the tested fuels were also measured. It is found that increasing ozone concentration in the oxidizer stream dramatically increased the reactivity of both fuels. The influence of fuel stream temperature on fuel ignition concentration has been examined. Results showed that an increase in fuel reactivity as fuel stream outlet temperature increases. Finally, with the aid of molecular transport and detailed chemistry, a numerical analysis was carried out to simulate the ignition and extinction of butane isomers cool flame; and to discuss the fidelity of chemical kinetics model to describe the butane isomers cool flame in diffusive systems. The results revealed that ignition and extinction limits of cool flames are predominantly governed by LTC. The model captured the trends in the experiments for both fuels. However, it overpredicted both ignition and extinction limits at all strain rates and ozone concentration. Sensitivity analyses were carried out to understand the reactions responsible for the ignition and extinction.
Experiments on the Breakup of Drop-Impact Crowns by Marangoni Holes

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Understanding the physics of a drop impact on a liquid surface is a growing area of interest for a wide variety of applications. One that is of special interest is in the internal combustion engine, as tiny droplets that hit the lubricant in the interior walls of an engine can directly affect the efficiency of the lubricating fluid. Moreover, depending on the impact energy, the lubricant may form secondary droplets that can harm the combustion efficiency.

Our research studies the breakup phenomenon of a high-viscosity drop impacting on a thin film of low-viscosity liquid, which also has lower surface tension, s. The thin film effectively produces free slip of the drop liquid along the solid and makes it deform into a prominent crown shape. Previous experiments [1] proposed that the breakup of the crown resulted from a spray of fine droplets ejected from the thin film.

These droplets hit the interior of the crown, forming spots with lower surface tension, driving the hole formation. The validity of such assumption is tested using close-up imaging to identify individual spray droplets. The footages show how the fine droplets hit the crown and influence the hole formation. We therefore conclude that the breakup is indeed due to Marangoni instability. To further investigate this, we have varied three main parameters: the viscosity of the drop μd, the surface tension of the thin film and thereby the strength of Ds and finally the thickness of the film d on the solid surface. Throughout the impact experiments, the release height is kept constant at H = 5.4 m, leading to an impact velocity of U = 9.5 m/s on the thin liquid film.
Valorization and Solidification of Fly Ash Collected from Power Plant Using Thermal Plasma

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The fly ashes treated in this work are collected from the power plants using heavy fuel oils in Saudi Arabia. The fly ash was analyzed by many technics such as X-ray fluorescence, CHN analyzer, inductively coupled plasma, and scanning electron microscopy. With these technics the composition, the chemical and physical proprieties of fly ash are determined. The results obtained by these analysis show that the fly ash mainly composed of carbon, and it contains also sulfur and metals such as V, Ca, Mg, Na, Fe, Ni, and Rh. The SEM analysis shows that fly ash particles are porous, have very irregular shapes and various particle sizes (20-50 μm). The valorization of fly ash consists of separation of metals from carbon and sulfur. For this reason, in the first step the fly ash was treated by pyrolysis/combustion plasma system to reduce the weight of carbon. Whereas for the solidification of fly ash, the product obtained by the combustion of fly ash was vitrified in a plasma furnace.

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Environmental contamination is a real threat affecting the environment and organisms. Air pollution has increased markedly as a result of growth in human activities and increased petroleum use for electricity generation, transportation, and industrial application. This has led to a significant rise in emissions that exceed international regulation limits. Internal combustion engines play a significant role in society’s health and power needs. However, the automobile is considered as the main source of pollution as well as of NOX emissions. This work presents a study of performance and exhaust emissions of internal combustion engine fueled by Saudi Arabian market gasoline RON91/RON95 with admixture of syngas and 5 % pure Ethanol (E5). Entirely automated engine and plasma converter system is developed to be fed with the same type of fuel. The engine is modified to make it run more efficiently by introduction of plasma based fuel reformer. Syngas is generated by partial oxidation of gasoline with air in plasma assisted fuel converter in present of steam to reduce the amount of soot produced in a plasma reactor. The fuel consumption and its related emissions are detected and experimental results obviously demonstrate essential total reducing of NOx engine emissions compared to original engine. The most obvious reducing of harmful pollutions is observed for lean conditions – about 50% reduction -. Meanwhile total gasoline consumption (including gasoline needed for plasma-assisted converter) slightly increased. Results also shows that NOx content for these new blends is lower for the using of E5-gasoline 91 comparing to E5-gasoline 95 and is lower in general for using E5-gasoline 91 and syngas than the E5-gasoline 95 and syngas.
Figure 1: NOx Emissions for ES-Gasoline 95 at Different Lean Mixtures and 2700 rpm

Figure 2: Fuel Consumption for ES-Gasoline 95 at Different Lean Mixtures and 2700 rpm

Figure 3: NOx Emissions for ES-Gasoline 91 at Different Lean Mixtures and 2700 rpm

Figure 4: Fuel Consumption for ES-Gasoline 91 at Different Lean Mixtures and 2700 rpm
Factors Affecting Cenosphere Morphology in HFO Single Droplet Combustion

Abdulrahman Alkhateeb, Ayman M. Elbaz, Jianguo Du, William. L. Roberts

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To better understand cenosphere formation and differences between two types of cenosphere morphologies in HFO combustion. Two different experiments of single Heavy Fuel Oil (HFO) droplet combustion inside preheated furnaces were done under a series of conditions and particulate matters were collected from the cooled exhaust gas. By using SEM and recording high speed images, morphology of cenosphere samples can be characterized. Results show that air co-flow rate and burning zone temperature inside furnace are the two main factors that affect the morphology of cenospheres. The morphology changes from porous shell to skeleton-membrane if air co-flow rate decreases from 150 lpm to 30 lpm or if burning zone temperature decreases from 600 C to 250 C. Relatively high temperature and high air co-flow rate are both required to generate cenospheres with porous shell structure.
The Feasibility Analysis of Supercritical Methane Recuperated Brayton Cycle Using GT-SUITE

Aibolat Dyuisenakhmetov, Robert Dibble

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The Supercritical CO$_2$ Recuperated Brayton Cycle (RCB) has gained attention as a possible alternative to Organic Rankine Cycle as a bottoming cycle for waste heat recovery. The efficiency and work output of RCB strongly depend on expander and compressor efficiencies and the specific ratio of heat capacities of a working fluid. The energy sector, for power output from tens of kW to several MW, is dominated by internal combustion reciprocating engines which are known to have a high isentropic efficiency. Basic calculations show that methane is efficient as carbon dioxide. The performance of Supercritical Methane RCB cycle using piston engines is analyzed using GT-SUITE software program.
High Pressure Soot Sampling in a Laminar Coflow Nonpremixed Flame

Anthony Bennett, Emre Cenker, William Roberts

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Soot formation is an important topic in combustion due to the detrimental effects soot has on human health and the environment. To understand the formation of soot in combustion environments, various optical diagnostic techniques have been applied and validated in atmospheric flames. To further extend our understanding of soot formation, experiments performed at pressures similar to those found in practical combustors are required. While optical diagnostic techniques may be used in these conditions, it is important for these diagnostics to be validated. To this end, a soot sampling device has been designed to obtain soot samples at high pressure. The design, based on (Leschowski, Dreier et al. 2014), uses a pneumatic cylinder to insert a TEM grid into the flame to capture soot particles thermophoretically. One of the main challenges with sampling soot under pressure is that the pneumatic devices use pressure to actuate. Thus, high pressure on the opposing side will prevent the pneumatic sampler from working properly. To overcome this, a sealing chamber is employed to separate the pneumatic piston from the pressure vessel. This allows the pneumatic piston to work even when pressure on the opposing side is much higher.

To determine the effects of pressure on soot morphology, soot sampling will be performed in a non-premixed laminar flame with an air coflow at various pressures from 1 to 20 bar. Samples will be obtained on carbon coated TEM grids and soot morphology will be analyzed using transmission electron microscopy (TEM). Effects of pressure on primary particle size, aggregate size and lattice structure will be reported.

High Temperature Rate Constants Measurements of OH Radicals with 1,2,3-Trimethyl-Benzene in a Shock Tube

Dapeng Liu, Fethi Khaled, Binod Giri, and Aamir Farooq*

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Reaction with hydroxyl radical (OH) is an important fuel consumption pathway at both combustion and atmospheric conditions. Rate constants for the reaction of OH with 1,2,3-trimethyl-benzene have been measured at high temperatures (900 – 1300 K) in a shock tube facility. The narrow line-width absorption OH at the R1(5) transition in the UV region is used to trace the OH concentration change. The UV beam is generated by frequency doubling of the ring-dye cw laser’s visible output at 613.37 nm light, which is powered by a 532 nm He-Ne laser. Five piezoelectric PCB transducers placed along the last section of the shock tube determine the incident shock velocity, the extrapolation of which is then used to determine pressure and temperature of the reflected shock wave. Interference absorption from aromatic radicals is observed under experimental condition. This interference is corrected to calculate the target rate constants.
Flame Front Insights at Extreme Combustion Conditions

Efstathios-Al. Tingas, Nurzhan Mukhadiyev, Hong Im

Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Understanding highly turbulent flames has been gaining a lot of practical interest recently, as the modern combustion devices, which aim to achieve higher efficiencies and lower emissions, are designed to operate at high-pressure, ultra-lean, low-temperature conditions. However, the processes that are involved in turbulent premixed combustion are considerably complex and some of the factors affecting it are so vague that our comprehension and description of this significant phenomenon is still poor. Therefore, the investigation of the interaction between turbulent flow and premixed flame at extreme combustion conditions becomes more challenging. To this end, various methods have been proposed.

One recently developed method that provides detailed information about the role of the processes in any reacting system is the Tangential Stretch Rate (TSR) approach. This method uses fundamental concepts and tools from the Computational Singular Perturbation (CSP) method framework, which allow to identify the cause-effect relationships between the action of the driving chemical processes and the reaction of the flow. As opposed to all other techniques, the TSR approach offers significant advantages such as: (i) identification of flame fronts (ii) identification of the most important processes (reactions or transport-related processes) both upstream/downstream and at the flame front (iii) determination of the front propagation mechanism, i.e., deflagration or ignition front. This technique has been successfully tested against spatially both homogeneous (batch reactors) and non-homogeneous systems.

In the current study, TSR analysis was conducted on two sets of direct numerical simulations (DNSs) that have been previously performed by Arias et al (Bull. Am. Phys. Soc., 60). The simulations were initialized with a laminar, premixed H2/air flame with equivalence ratio of 0.7, using the detailed chemical mechanism by Burke et al (Int. J. Chem. Kinet, 44(7), 444–474). The computational parameters for Case 1 were Re=227, Ka=0.75, Da=20 and for Case 2 were Re=1623, Ka=14.4, Da=5. At every time instant, the flame front was identified as the region where the TSR variable turned negative. In both cases, the dominant role of kinetics was confined to a thin region at the tip of the flame front, similarly to what has been found at the laminar case, indicating that the flame propagation mechanism was a spontaneous ignition front. Finally, the dominant kinetics scheme was identified an the role of the chain branching reaction H + O2 => H + O2 was highlighted.
Numerical Simulation of the Influence of Partial Premixing on the Propagation of Partially Premixed Flames

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Department of Mathematics, Taif University, Taif, Saudi Arabia

This paper examines the influence of a partial premixing between the reactants prior to the reaction on the structure and propagation of triple flames formed in a mixing layer. The problem has been mathematically formulated in the framework of the thermo-diffusive model under a single-step irreversible chemical reaction. A computational modelling and numerical simulations based on finite elements were then employed to solve the governing equations. The study has shown that the flame structure and characteristics such as its speed, maximum temperature were significantly modified in the presence of premixing. The triple Flame structure were found to exhibit several changes such as: the shift of the leading edge toward the combustion mixture side, the weakening of the upper premixed branch, and the increase in the flame area. It has been predicted that the premixing can substantially enhance the reactivity of the combustion mixture, but on the other hand it tends to shift the flame to the boundary which may destroy the combustion chamber.
Multi-Angle Light Scattering in a Counterflow Flame at Elevated Pressures

Hafiz Muhammad Fahid

Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Practical combustion devices are designed to operate at high pressures to optimize their efficiency and size. But increase in pressure significantly increases the overall soot yield. These emissions are harmful to environment and human health. The airborne lifetime of soot particles and their interaction with human respiratory system depend on their morphology. A better understanding of how the soot is formed and oxidized is a key to control its overall emissions. In this work, different morphological parameters of soot are investigated using multi-angle light scattering and extinction, at elevated pressures. An $N_2$-diluted ethylene/air counterflow diffusion flame is stabilized inside the pressure vessel, up to 5 atm. The pressure vessel has four optical windows and can provide the optical access for multi-angle light scattering from 10 to 165 degrees. An Ar/Kr ion laser beam emitted at 514.5 nm wavelength is focused at the center of the flame and light scattered by soot particles is collected by light collection optics that are mounted on a rotary stage. Global strain rate of 30 s$^{-1}$ is maintained constant at all pressures. The scattering measurements are analyzed using Rayleigh-Debye-Gans theory for polydisperse fractal aggregates and information about soot concentration, mean particle diameter, aggregate size distribution and fractal dimension is inferred up to 5 atm.

Figure: Schematic of laser diagnostic for multi-angle light scattering

PD = Photo detector
LLF = Laser line filter
IS = Integrating Sphere
RB = Reference beam
PMT = Photo multiplier tube

J. Masurier, M. Waqas, B. Johansson

Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

The present poster will introduce the work-in-progress on the Cooperative Fuel Research (CFR) engine available here in KAUST. Up to now, the engine was running under spark ignition (SI) conditions for RON and MON tests as well as under HCCI conditions for autoignition tests. However, experimental conditions are limited with this CFR engine. Thus, we aim to upgrade this experimental setup in order to reach wider operating ranges and to get more impact of our research on fuels.

To achieve these objectives, we modified the intake of the CFR engine. Now, the flow of air inducted by the engine is controlled by a mass flow controller (MFC) that enables us to reach a wide range of intake pressures. Other MFCs are also used to control the fuel. A set of six liquid MFCs can controlled independently the injection rate of different pure fuels, meaning that we are able to customize mixture of fuel and to study a wide range of equivalence ratio. Moreover, other parameters such as the intake temperature and the rotation speed are extended to reach maximum value of 200 Celsius degrees and 1500 rpm, respectively. Then, based on this brand-new version of the CFR engine, we integrated an automated control that enable us to run experiments with a robust strategy.

Finally, this experimental setup helps us to generate rapidly data for investigating different topics related to the fuels, such as the blending octane numbers and/or the low temperature heat release. Some of the results already obtained will be presented in the present poster.
Thermal Properties of Heavy Fuel Oil

Khalid Al-Qurashi, Ayman Elhagrasy, William Roberts

Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

There is an increasing interest in the comprehensive study of heavy fuel oil (HFO) due to its growing use in furnaces, boilers, marines, and recently in gas turbines. In this work, the thermal properties and chemical composition of HFO are presented. Two HFOs from different locations were considered. Thermogravimetric analysis (TGA) was performed to study the nonisothermal HFO decomposition behavior. The results showed that both fuels exhibited similar thermal decomposition. The thermal properties also probed information about the boiling point range of each fuels. The results suggested that these fuels may exhibit similar combustion characteristics.

### Table 1. HFO physical properties and elemental composition

<table>
<thead>
<tr>
<th>Physical properties</th>
<th>Method</th>
<th>Units</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density at 288 K</td>
<td>ASTM D 4052-11</td>
<td>Kg/m³</td>
<td>970.5</td>
</tr>
<tr>
<td>Specific gravity (60/60°F)</td>
<td>ASTM D 4052-11</td>
<td>-----</td>
<td>0.9711</td>
</tr>
<tr>
<td>Kinematic viscosity at 40°C</td>
<td>ASTM D 445-12</td>
<td>cSt</td>
<td>617.740</td>
</tr>
</tbody>
</table>

### Compositional data

<table>
<thead>
<tr>
<th>Elemental content</th>
<th>Method</th>
<th>Units</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sulfur</td>
<td>ASTM D 4294-10</td>
<td>mass%</td>
<td>3.292%</td>
</tr>
<tr>
<td>Asphaltene content</td>
<td>IP 143</td>
<td>Wt%</td>
<td>8.2%</td>
</tr>
<tr>
<td>Vanadium</td>
<td>IP 501-05</td>
<td>mg/Kg</td>
<td>18.0</td>
</tr>
<tr>
<td>Nickel</td>
<td>IP 501-05</td>
<td>mg/Kg</td>
<td>11.0</td>
</tr>
<tr>
<td>Sodium</td>
<td>IP 501-05</td>
<td>mg/Kg</td>
<td>3.4</td>
</tr>
<tr>
<td>Zinc</td>
<td>IP 501-05</td>
<td>mg/Kg</td>
<td>&lt;1.0</td>
</tr>
<tr>
<td>Lead</td>
<td>IP 501-05M</td>
<td>mg/Kg</td>
<td>0.4</td>
</tr>
<tr>
<td>Potassium</td>
<td>IP 501-05M</td>
<td>mg/Kg</td>
<td>0.1</td>
</tr>
<tr>
<td>Carbon</td>
<td>EPA 440.0</td>
<td>mass%</td>
<td>85.0%</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>EPA 440.0</td>
<td>mass%</td>
<td>10.89%</td>
</tr>
<tr>
<td>Oxygen</td>
<td>EPA 440.0</td>
<td>mass%</td>
<td>0.030%</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>EPA 440.0</td>
<td>mass%</td>
<td>0.239%</td>
</tr>
</tbody>
</table>

### Heating Values

<table>
<thead>
<tr>
<th>Heating Value</th>
<th>Method</th>
<th>BTU/lb</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Higher heating value</td>
<td>ASTM D 4868</td>
<td></td>
<td>18258</td>
</tr>
<tr>
<td>Lower heating value</td>
<td>ASTM D 4868</td>
<td></td>
<td>17255</td>
</tr>
</tbody>
</table>
Octane Number Prediction Using Artificial Neural Network

Khalid Al-Qurashi¹, Belkacem Kada², William Roberts¹

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²Department of Aeronautical Engineering, King Abdulaziz University, Jeddah, Saudi Arabia

Octane number (ON) is a means to study the ignition quality of gasoline fuels. The ON is qualitatively measured in cooperative fuel research (CFR) engines in accordance to ASTM D-2699 and ASTM D-2700. However, the CFR measures are complex, expensive, and not accessible to many research institutes. With the fact that ON does not blend linearly in most cases, we propose the development of an accurate and robust predictive model to estimate the ON of gasoline-like fuels at variable ignition conditions using advanced Artificial Neural Network (ANN) algorithms. The training data for the ANN were derived from CHEMKIN. Primary reference fuels (PRF) and ternary reference fuels (TRF) were used as gasoline surrogates in CHEMKIN. The variable parameters considered in this research are ON, pressure (P), temperature (T), and equivalence ratio (φ). The ranges of ON, P, T, and φ are 80 to 100, 10 to 40 bar, 550 to 1200 °C, and 0.5 to 1.5, respectively. The ignition delay (τig) in this research is used as the ON predictor. From the ANN, the ON can be predicted for any surrogate fuels by providing τig, P, T, and φ. In addition, the ANN algorithm shows the effects of nonlinear blending properties upon both τig and ON.

<table>
<thead>
<tr>
<th>Variables</th>
<th>Min value</th>
<th>Max value</th>
<th>Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>P [bar]</td>
<td>10</td>
<td>39</td>
<td>0.3</td>
</tr>
<tr>
<td>T [°C]</td>
<td>550</td>
<td>1200</td>
<td>6.5</td>
</tr>
<tr>
<td>ON</td>
<td>80</td>
<td>100</td>
<td>2</td>
</tr>
</tbody>
</table>
Effect of Base Fuel Composition on Ethanol Blending Octane Number

Muhammad Waqas, Nimal Naser, Mani Sarathy, Kai Morganti, Khalid Al-Qurashi, Bengt Johansson

Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Future internal combustion engines demand higher efficiency, progression towards which is limited by antiknock quality of present fuels and energy economics in octane enhancement. A possible solution is Octane-on-Demand, that uses a combination of high and low octane fuels in separated tanks to create fuels of the required octane rating according to demand. Ethanol with a RON 107 was selected as the high RON fuel and three low octane fuels were used as base fuel. These were for the FACE (Fuels for Advanced Combustion Engines) study, more specifically FACE I, J and A but also primary reference fuels (iso-octane/n-heptane) were used.

A CFR engine was used to conduct the experiments. For SI combustion the CFR was operated at RON conditions that correspond to engine speed of 600 rpm and air inlet temperature of 52 oC. The engine was also operated in HCCI mode to get the auto ignition properties at lean conditions. The engine was then operated in four conditions, similar to the RON and MON cases to obtain four HCCI numbers.

The octane numbers corresponding to four HCCI fuel numbers and the RON were obtained for a concentration of ethanol of 0, 2, 5, 10, 15 and 20%. It was found that the increase of octane number of ethanol was not linear with percentage added. This means that the effective octane number of ethanol, or the blending octane number, changed from close to 200 with a small percentage down to a number closer the that of ethanol, 107 with larger quantities. The base fuel composition played a significant role for the blending octane number of ethanol. Both base fuel octane number and composition mattered. Heat Release analysis are shown to further explain these conclusions.
A Computational Study on the Effect of Oxidation Pathways on Soot Formation in Diffusion Flames

Prabhu Selvaraj, Hong G Im
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Particle oxidation is one of the steps still not completely understood in combustion. Most of the approaches are based on semi-empirical reaction rates. Correct evaluation of oxidation is needed to predict the final emission of particles in diffusion flames. Two counterflow diffusion flames have been chosen, a soot formation (SF) and a soot formation/oxidation (SFO) flame. The impact is more sensitive in the case of SFO flames due to the importance of the oxidation pathway. In SFO flame, the volume fraction decreases approaching the oxidation zone, suggesting that soot oxidation is effective. The mean diameter remains very small suggesting that together with the surface oxidation, fragmentation process is activated. The two principal soot oxidizers in flames are the hydroxyl radical (OH) and molecular oxygen (O2). Many soot oxidation rate expressions exist for these oxidizers. But there is considerable disparity and uncertainty in the existing soot oxidation rate models for OH and O2. Thus motivated, the objective of this study is to compare the existing rates and optimize soot oxidation rate expressions for OH and O2 in diffusion flame. A reduced mechanism with PAH pathways until coronene and MOMIC method has been employed in Cantera to calculate the soot characteristics of counterflow diffusion flame. Simulation results are compared with the experimental data obtained from SFO flames and also the influence of various strain rates have been analyzed.
Propagating Behaviors of Twin Premixed Edge-Flames under DC Electric Fields

Sung Hwan Yoon, Min Suk Cha

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Twin premixed edge-flames in a counterflow, annular slot burner were studied to examine effects of direct current (DC) electric fields. As DC was applied to a lower part of the burner and the upper was grounded, generated electric field lines were perpendicular to the direction of edge-flame propagation. Generally, a bulk motion generates due to a momentum transfer from charge carriers to neutral molecules called as ionic wind, thereby, the flow field could be changed. In this respect, three distinct types of edge-flame behaviors were experimentally identified in electric field; (1) reduced displacement speeds at low strain, (2) enhanced displacement speeds at high strain and (3) retreating edge-flames at high strain. Also, effects of electric field on ignitable range were estimated that low strain ignitable limits shrank and high strain ignitable limits expanded with applied voltages comparing with those of no electric field. Finally, we described coupling effects between premixed flame propagation and electric fields based on measured twin premixed edge-flame speeds with various strain rate.
A Graphical User Interface for Model Reduction of Complex Fuels Based on Principal Component Analysis and Artificial Neural Networks

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Department of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, USA

A graphical user interface (GUI) for model reduction of complex fuels is developed. The GUI is based on principal component analysis (PCA) for model reduction and artificial neural network (ANN) for the reconstruction of thermo-chemical scalars. The target complex fuels’ chemical mechanisms are characterized by hundreds or thousands of chemical species and thousands or tens of thousands of chemical reactions. An account for the detailed chemistry of such fuels computationally is expensive. The GUI is designed to generate a significantly-reduced set of scalars, principal components (PCs) that describe the complex composition space originally represented by the full set of thermo-chemical scalars. The approach is a viable alternative to chemistry reduction schemes and may be used in combination with these schemes. The GUI is built with many features that enable the selection of a subset of the thermo-chemical scalars for PCA, the determination of the number of PCs that reproduce the original scalars’ variance, the evaluation of chemical source terms and diffusion coefficients of the PCs and the generation of visual and mechanisms for exporting the GUI output for validation and implementation in computational codes. Validation of the GUI is presented to illustrate its performance.

Keywords: 1) Low-dimensional manifolds, 2) principal component analysis.
Dynamics of Lean Premixed Hydrogen/Air and Syngas/Air Flames behind a Meso-Scale Bluff-Body

Yu Jeong Kim, Bok Jik Lee*, and Hong G. Im

Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Bluff-bodies have been used as effective flame holders for practical applications of premixed flames, such as gas turbine engines. While many studies about bluff-body stabilization have been done both experimentally and numerically, it is still necessary to understand flame stabilization mechanism on a meso-scale bluff-body. In the present study, flame dynamics are investigated using high fidelity simulations with a full temporal and spatial resolution. Direct numerical simulations are conducted to investigate dynamics of lean premixed hydrogen and syngas flames behind a meso-scale bluff-body by increasing the inflow velocity, as a key hydrodynamic parameter, up to blowoff limit. A two-dimensional domain of 10 mm by 10 mm with a square-shaped bluff-body holder of 0.5 mm is considered. Flame dynamics are observed by increasing the mean inflow velocity from a stable state to blowoff. Several distinct flame behaviors are identified as the inflow velocity increasing until blowoff occurs, such as steadily stable, mild fluctuation on the shear layer, symmetrical vortex-shedding, asymmetrical vortex shedding, and vortex street. At the near-blowoff, the intermittent transition of a combination of symmetrical and asymmetrical shedding was temporally observed, then the ultimate extinction occurs, showing the vortex-street. The objective of this study is understanding of what causes the total blowoff of the flame. The detailed temporal evolutions and phenomenological observations are compared between two mixtures and discussed in detail.

![Figure. Instantaneous snapshots of iso-contours of heat release rate in hydrogen/air mixture as increasing the inflow velocity (U) until blowoff occurs.](image-url)
Sooting Limit in Non-premixed Counterflow Flames of Ethylene with Dimethyl Ether Addition

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Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Dimethyl ether (DME) is regarded as one of the most promising alternative fuels because of the positive role that DME played in the reduction of combustion emissions, such as NOx, SOx, and soot particles. Previous studies have evaluated the synergistic effect of dimethyl ether as a substituent on soot formation in counterflow ethylene flames. They revealed that a small amount of DME addition would enhance soot formation, while further increase of DME would inhibit soot formation.

In this work, a systematic investigation of sooting limits was developed in counterflow diffusion flames of DME and ethylene mixtures. The synergistic effect mentioned above was highlighted. Laser extinction and scattering technique was conducted to evaluate the critical fuel mole fractions ($x_{f,cr}$) and critical oxygen mole fractions ($x_{o,cr}$) at the point that soot start to appear in the elastic light scattering signal. Based on the $x_{f,cr}$ and $x_{o,cr}$, sooting limit map of ethylene/DME mixtures was draw with the DME mixing ratios ($\beta$) ranging from 0% to 50% of the total carbon fed. Flames of a higher DME adding showed a lower propensity for sooting when $\beta>5\%$, while flames of a higher DME adding led to a higher sooting propensity when $\beta<5\%$. Additionally, sooting temperature index was introduced to rate sooting trend of DME doping ethylene flames and a similar synergistic effect of DME addition was found. The limiting flame temperatures were computed using Chemkin. To explain the possible mechanism for the experimental results, numerical simulations were performed to analyse the concentration distributions of several crucial species (CH$_3$, C$_2$H$_2$, C$_3$H$_3$, OH and benzene) in ethylene flames with different DME additions.
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