Role of Combustion Research in Circular Carbon Economy

Saudi Arabian Section of the Combustion Institute

Eleventh Annual Meeting

Jointly organized by the Transport Technologies R&D Division of Saudi Aramco and the Clean Combustion Research Center at King Abdullah University of Science and Technology (KAUST)

12th-13th, October 2021

Saudi Arabian Section of the Combustion Institute

Contents

Welcome

Welcome to the 11th Saudi Arabian Section of the Combustion Institute (SAS-CI) Annual Meeting. The theme of the event will be *Role of Combustion Research in Circular Carbon Economy*.

In its comparatively short history, the Saudi Arabian Section has grown in both size and stature. The Section has more than 180 registered members in Kingdom. But more importantly, the annual meeting has increasingly been attracting high-profile international researchers. We expect the growth in both local and international participation will continue its upward trajectory in future years as we contribute to tackle the challenges and hopes that combustion represents for the future of world energy mix.

The Eleventh Annual Meeting will be held online on October 12-13, 2021 due to the continuing COVID-19 pandemic situation. Nevertheless, collectively, the meeting will feature four keynotes and 53 oral presentations across eight different technical sessions which we believe will be a great opportunity for our community to continue building and sharing knowledge unconditionally.

From the organizers, we hope you enjoy the event.

Abdullah AlRamadan *Saudi Aramco*

Fethi Khaled *Saudi Aramco*

Aamir Farooq *King Abdullah University of Science and Technology*

Saudi Arabian Section of the Combustion Institute Leadership

Chairman

Prof. Hong Im *King Abdullah University of Science and Technology*

Vice-Chairman

Dr. Jihad Badra *Saudi Aramco*

Secretary

Ms. Maryam Altaher *Saudi Aramco*

Officers

Prof. S. Mani Sarathy *King Abdullah University of Science and Technology*

Prof. William Roberts *King Abdullah University of Science and Technology*

Dr. Amer Amer *Saudi Aramco*

General Event Information

The 11th SAS-CI meeting is a held online due to the continuing Covid-19 pandemic situation.

The following information will assist you to connect to this virtual event. **Zoom** online meeting was chosen as the platform for this event.

The event will feature two parallel rooms:

ROOM 1: the main room of the event and will feature the welcome notes, the keynotes' presentation and the first session agenda

Link of ROOM 1: https://kaust.zoom.us/j/91789450817

ROOM 2: the parallel room of the event and will feature the second session agenda.

Link for ROOM 2: https://kaust.zoom.us/j/96299636036

How to connect to the online meeting?

1- Ensure you have decent speed internet connection
2- Ensure you have ZOOM installed in your smartphone, laptop or desktop. Alternatively, you can connect to zoom directly through your browser from your desktop
3- On the day of the event, press the links of either rooms: ROOM 1 or ROOM 2 depending on which session you want to attend. Note that the links will only work during the official time of the 11th SAS-CI meeting event.
4- If you are a presenter and during the time slot allocated to your presentation, you will be automatically upgraded as a panelist to be able to share your screen and use the microphone.

Technical Issues Contacts

Please contact Fethi (+966 59 194 9287) or Abdullah (+966 50 583 3244) if you have any question or if you encounter any difficulty accessing the virtual event.

Session Chairs

Session 1.1: Applications of ML/AI tools

Jihad Badra *Saudi Aramco*

Session 1.2: Low carbon fuels and CCUS

Tamour Javed *Saudi Aramco*

Session 2.1: Fundamental combustion research, measurement techniques and modelling

Thibault F. Guiberti *KAUST*

Session 2.2: Engines and power generation systems with lower carbon footprint

Deanna Lacoste *KAUST*

Session 3.1: Hydrogen and ammonia as energy carriers

Christos Kalamaras *Saudi Aramco*

Awad Alquaiti *KFUPM*

Session 3.2: Air quality and fuel criteria pollutants

Gaetano Magnotti *KAUST*

Session 4.1: Combustion measurement techniques, diagnostics and emissions

Emre Cenker *Saudi Aramco*

Session 3.1: Combustion and reaction kinetics

Abdul Gani Abdul Jameel *KFUPM*

Program

1. Tuesday, October 12th (Morning)

Time Zone: Saudi Arabia Time (Riyadh, UTC+03:00)

8.00 – 8.15	**Login Phase**	
8.15 – 8.30	**Welcome – SASCI Chairman, Prof. Hong Im, KAUST**	
8.30 – 9.30	**Invited Speaker – Mr. Yehia Khoja, Ministry of Energy:** The circular carbon economy national program, the energy innovation program, and the AI center for energy to unlock additional value from the energy sector	
9.30 – 9.40	**Short Break**	
9.40 – 12.10	**Session 1.1: Applications of ML/AI tools** *Session Chair: Dr. Jihad Badra, Saudi Aramco*	**Session 1.2: Low carbon fuels and CCUS** *Session Chair: Dr. Tamour Javed, Saudi Aramco*
9.40 – 10.00	Data-driven prediction of flame lift-off-length and ignition delay of ECN spray-A *Balaji Mohan, Saudi Aramco*	The future of direct air capture at NEOM *Yasmeen Najm, NEOM*
10.00 – 10.20	A transfer learning approach to multi-target temperature-dependent reaction rate prediction *Emad Al Ibrahim, KAUST*	Analysis of methane, propane, and syngas oxy-flames in a fuel-flex gas turbine combustor for carbon capture *Medhat Nemitallah, KFUPM*
10.20 – 10.40	Fuel design using genetic algorithm and artificial neural networks *Faisal Albaqami, KFUPM*	Mobile carbon capture for marine applications: An MDEA/PZ solvent process model case scenario *Fethi Khaled, Saudi Aramco*
10.40 – 10.50	**Short break**	
10.50 – 11.10	Machine learning model for gasoline compression ignition at low loads *Zahra Al Ibrahim, Saudi Aramco*	Doping effect of oxygenated and non-oxygenated bio-oils on non-premixed turbulent hydrogen-based flames *Yilong Yin, University of Adelaide*
11.10 – 11.30	A machine learning surrogate approach for the optimization of fuel-engine design *Mohammed Almomtan, KAUST*	A decoupling model approach to studying the pyrolysis and oxidation of C6-C10 saturated fatty acid methyl esters (FAMEs) *Xiaoyuan Zhang, KAUST*
11.30 – 11.50	Utilization of machine learning to predict the products' yields from co-pyrolysis of biomass and polymers *Aessa Alabdrabalnabi, KAUST*	Effect of exhaust gas recirculation (EGR) and ethanol addition on ignition delay Times of Gasoline Fuels *Khalid Aljohani, KAUST*
11.50 – 12.10	Large eddy simulation with flamelet progress variable approach via neural network acceleration *Lorenzo Angelilli, KAUST*	High-temperature mid-IR absorption and kinetic study of the dioxolanes *Mohammad Adil, KAUST*
12.10– 13.10	**Lunch Break**	

2. Tuesday, October 12th (Afternoon)

Time Zone: Saudi Arabia Time (Riyadh, UTC+03:00)

13.10 – 14.10	**Invited Speaker – Prof. Bassam Dally, KAUST:** New insights into laminar and turbulent sooting flames	
14.10 – 14.20	**Short break**	
14.20 – 16.50	**Session 2.1: Fundamental combustion research, measurement techniques and modelling** *Session Chair: Prof. Thibault F. Guiberti, KAUST*	**Session 2.2: Engines and power generation systems with lower carbon footprint** *Session Chair: Prof. Deanna Lacoste, KAUST*
14.20 – 14.40	Minimum ignition energy measurement of methane-air at cryogenic conditions *Anupam Ghosh, KAUST*	Fuel economy assessment of modern engine technologies in a range-extended electric vehicle *Emre Cenker, Saudi Aramco*
14.40 – 15.00	Direct numerical simulations of super-knock development process in IC-engine conditions *Minh Bau Luong, KAUST*	An unconventional internal combustion engine as a range extender for low carbon mobility *Giovanni Vorraro, KAUST*
15.00 – 15.20	Numerical study on NOx formation in premixed turbulent C3H8-air flames diluted with CO2-H2O, *Hemaizia Abdelkader, University of Sciences and Technology Houari Boumediene*	Ignition regimes of GCI engines and the usefulness of autoignition surrogates for GCI fuels with varying sensitivities *Jihad Badra, Saudi Aramco*
15.20 – 15.30	**Short break**	
15.30 – 15.50	Autoignition experiments of iso-octane at ultra-lean and lean conditions *Khayyom Hakimov, KAUST*	Numerical evaluation of cold operation strategies in a heavy-duty gasoline compression ignition engine *Emma Zhao, Aramco Services Company*
15.50 – 16.10	Numerical study of lean premixed humidified hydrogen-methane-air combustion in a generic triple swirl burner *Neha Vishnoi, Indian Institute of Technology Ropar*	A computational investigation of the combustion behavior and turbulence-chemistry interaction in a narrow-throat prechamber combustion engine *Mickael Silva, KAUST*
16.10 – 16.30	Active control of thermoacoustic instabilities in a premixed laminar flame using time phased bursts of nanosecond repetitively pulsed discharges *Ammar Alkhalifa, KAUST*	A priori computational assessment of laminar flame speed correlation in an ultralean prechamber engine *Ghufran Alkhamis, KAUST*
16.30 – 16.50		Multiple injections to enable fuel flex engines *Bassam Aljohani, KAUST*
16.50	**End of first day**	

3. Wednesday, October 13th (Morning)

Time Zone: Saudi Arabia Time (Riyadh, UTC+03:00)

8.15 – 8.30	**Login Phase**	
8.30 – 9.30	**Invited Speaker – Dr. Umesh Patil, Air Products:** The true promise of H_2 in Saudi Arabia: Moving beyond the hype	
9.30 – 9.40	**Short Break**	
9.40 – 12.10	**Session 3.1: Hydrogen and ammonia as energy carriers** *Session Chairs: Dr. Christos Kalamaras, Saudi Aramco Prof. Awad Alquaiti, KFUPM*	**Session 3.2: Air quality and fuel criteria pollutants** *Session Chair: Prof. Gaetano Magnotti, KAUST*
9.40 – 10.00	Enhancing ammonia combustion by blending with diethyl ether *Binod Giri, KAUST*	Challenges on the road to zero-emission vehicles *Fakhar Mehmood, Saudi Aramco*
10.00 – 10.20	Experimental rig for hot ammonia nitridation studies *Nicole Laws, KAUST*	An interference-free laser-based methane sensor using cepstral analysis *Mhanna Mhanna, KAUST*
10.20 – 10.40	Oxidation of formic acid and decane using Jet Stirred Reactor *Shamjad Moosakutty, KAUST*	Experimental study on the Swirling Flame Combustion of Heavy Fuel Oil/Water Emulsion *Felipe Campuzano, KAUST*
10.40 – 10.50	**Short break**	
10.50 – 11.10	Hydrogen evolution from hydrocarbon pyrolysis in a simulated liquid metal bubble column reactor *Fabiyan Shamsudheen, KAUST*	Stability limits and emission performance of ammonia-methane swirl flames for future power generation *Marwan Abdullah, Saudi Aramco*
11.10 – 11.30	DNS of hydrogen flames at elevated pressures: turbulent flame speed analysis *Wonsik Song, KAUST*	Stability limits and emissions of double swirl burner with methane/ammonia blends *Alfaisal Albalawi, KAUST*
11.30 – 11.50	Hydrogen as a fuel for HCCI engines *Abdulrahman Mohammed, KAUST*	Experimental investigation of soot formation at elevated pressure in laminar inverse diffusion flames *Peng Liu, KAUST*
11.50 – 12.10	Characterization of a novel dual-fuel, dual-swirl burner for carbon free fuels *Amit Kotch, KAUST*	Soot formation in ammonia-hydrocarbon combustion *Peng Liu, KAUST*
12.10– 13.10	**Lunch Break**	

4. Wednesday, October 13th (Afternoon)

Time Zone: Saudi Arabia Time (Riyadh, UTC+03:00)

13.10 – 14.10	**Invited Speaker – Prof. Sophie Colson, Tohoku University:** Study of ammonia combustion fundamental characteristics	
14.10 – 14.20	**Short break**	
14.20 – 16.30	**Session 4.1: Combustion measurement techniques, diagnostics and emissions** *Session Chair: Dr. Emre Cenker, Saudi Aramco*	**Session 4.2: Combustion and reaction kinetics** *Session Chair: Prof. Abdul Gani Abdul Jameel, KFUPM*
14.20 – 14.40	Elucidating first stage ignition chemistry of dimethyl ether using a laminar flow reactor *Awad Alquaity, KFUPM*	On the accuracy of CO/H2 Kinetic Mechanisms for Prediction of Syngas Non-premixed Flames Characteristics *Syed Mughees Ali, Eindhoven University of Technology*
14.40 – 15.00	A step toward quantitative planar laser-induced fluorescence of hydroxyl radical in hydrogen-fueled detonations *Karl Chatelain, KAUST*	Surrogate formulation and chemical kinetic modeling of vacuum residual oil *Mohammed AlAbbad, KAUST*
15.00 – 15.20	Dual-camera high-speed imaging of ethanol combustion in a high-pressure shock tube *Miguel Figueroa Labastida, KAUST*	Global chemical kinetics of HFOs pyrolysis for practical applications *Elia Colleoni, KAUST*
15.20 – 15.30	**Short break**	
15.30 – 15.50	A laser diagnostic for HCN detection in mid-infrared *Ali Elkhazraji, KAUST*	Kinetic and product analysis of the pyrolysis of Salicornia bigelovii under CO2 and N2 atmospheres *Jinan Aljaziri, KAUST*
15.50 – 16.10	Characterization of a Cassegrain optical system for spatially-resolved measurements of flame chemiluminescence spectra *Amjad Aljarallah, KAUST*	Investigating 1, 3-butadiene kinetics using UV absorption spectroscopy *Dapeng Liu, KAUST*
16.10 – 16.30	Laser-induced fluorescence of NO in laminar and turbulent ammonia-hydrogen-nitrogen diffusion flames at high pressure *Guoqing Wang, KAUST*	-
16.30	**Closure of the 11th SAS-CI meeting**	

Keynote Presentations

1. Keynote I:

The Circular Carbon Economy National Program, the Energy Innovation Program, and the AI Center for Energy to Unlock Additional Value from the Energy Sector

Yehia Khoja
Advisor,
Ministry of Energy, Saudi Arabia

Abstract: The Saudi Ministry of Energy has been on a transformational journey to unlock additional value from the energy sector. This is done through ambitious programs in collaboration with partners in government, research, and industry. Some of these flagship programs include: the Circular Carbon Economy National Program, the Energy Innovation Program, and the AI Center for Energy. In this talk, we provide an overview on each of these efforts by describing their objectives, main initiatives, and the role that the Ministry of Energy plays to drive this transformation.

About the Speaker: Yehia Khoja is an Advisor at the Saudi Ministry of Energy, and an energy professional with over 10 years of experience covering energy system optimization, energy efficiency, local content development, circular carbon economy, artificial intelligence, and innovation. He has a proven record of leading teams in different energy programs involving stakeholders from government, research, and industry. He has helped develop Saudi Arabia's first set of industrial energy efficiency targets which helped achieve estimated savings of $1 billion dollars annually by 2030. Next, he led a team during the COVID-19 pandemic to localize the production of sanitizer raw materials by leveraging the existing companies in the energy sector. Currently, he leads three key and transformative initiatives at the Ministry of Energy: the Energy Innovation Program, the Artificial Intelligence Center for Energy, and the Energy Ecosystem Digital Transformation. He received his Master's degree in Electrical Engineering and his MBA from Stanford University, and his Bachelor's degree in Electrical Engineering from Purdue University.

2. Keynote II:

New Insights into Laminar and Turbulent Sooting Flames

Bassam Dally

Professor, Mechanical Engineering
King Abdullah University of Science and Technology, Saudi Arabia

Abstract: Soot in flames have been under intense investigation for many years, due to its impact on the environment (haze and acid rain) and public health (cancer and asthma) if emitted from flames. On the other hand, soot in flames enhances the thermal radiation, which in turns improve the thermal efficiency of combustion devices like furnaces and boilers. Consistent research has shown that the current soot models have failed to offer reliable predictions of soot inception and growth in turbulent flames and for practical fuels. Latest advances in laser-based measurement techniques have re-energized the quest for better soot models through systematic experimental studies into a variety of flames and fuels offering new insights and benchmark data. In this talk, the latest development in the planar measurements of temperature, soot volume fraction and primary soot particles' distribution will be presented. The talk will present results and findings from a variety of campaigns of sooting steady and forced laminar jet flames, Jet and bluff-body turbulent flames and jet in a hot coflow flames. A variety of fuels and blends will also be discussed. The talk will also provide some thoughts on future research needs.

About the Speaker: Bassam Dally is a Professor of Mechanical Engineering and a member of the Clean Combustion Research Center at KAUST.

Over the last 30 years, Prof Dally has contributed seminal works on a variety of research topics under the broad field of Thermo-Fluids. His major contributions are in turbulent reacting flows, MILD combustion, soot in flames, plasma propulsion, hybrid of concentrated solar thermal and combustion, and applied laser diagnostics. He has attracted millions of dollars for his research and have published more than 170 papers in leading scientific journals. He won many awards over the years, including 'Energy Professional of the Year in South Australia', and recently was awarded a Fellowship of the Combustion Institute.

3. Keynote III:

The True Promise of H2 in Saudi Arabia: Moving Beyond the Hype

Umesh Patil

R&D Manager,
Air Products Technology Center, Saudi Arabia

Abstract: Air Products is playing a major role in globally significant Blue and Green Hydrogen Development. There is a clear path for large-scale deployment of low-carbon hydrogen, as evidenced by our present projects in NEOM, Jubail and recently in Edmonton . However, for that to happen, the sector must focus on the appropriate applications of the technology—and there must be a legislative framework that encourages those applications while discouraging expenditures, especially in the technology areas where CCU efforts will not flourish. That is to say, everyone involved must get past the hype and focus on the true promise of hydrogen.

About the Speaker: Umesh has been the Air Products Technology Centres' R&D manager since 2018. He oversees Air Products' research collaboration activities in the Middle East, collaborating closely with major customers and universities. His technology team supports Air Products' business, operations, and joint ventures in Grey, Blue, Green hydrogen and Residue Gasification. Umesh holds both an M.S. and a Ph.D. in Materials Chemistry. He has spent the last ten years in Saudi Arabia working on technologies ranging from molecules to megawatts scale in the energy, petrochemical, and oil and gas sectors, with increasing responsibilities throughout his career.

4. Keynote IV:

Study of ammonia combustion fundamental characteristics

Sophie Colson

Specially Appointed Assistant Professor,
Institute of Fluid Science, Tohoku University

Abstract: Ammonia has attracted a lot of attention in recent years as a promising carbon-free energy carrier for the transition toward a greener society. Its combustion in thermal power stations enables electricity production without carbon emission, and while its production still heavily relies on hydrocarbons, it has the potential for the transition toward a cleaner energy production cycle, using gradually more blue and green ammonia, and limiting our CO2 emissions, as demonstrated by the Saudi Arabia blue ammonia shipping to Japan just a year ago. Its flexibility, affordability, and reliability make ammonia indispensable in tomorrow's energy sector and industry.

Though ammonia combustion has been studied for several years, some challenges still remain for the extension of this knowledge and for its broad deployment in a variety of applications.

In this presentation, some of the recent results obtained in the IFS, Tohoku University, on ammonia combustion fundamentals will be introduced, followed by a presentation of some upcoming research projects and future challenges.

About the Speaker: Sophie Colson received her Ph.D. in Aerospace engineering with a specialization in thermal energy from Tohoku University and INSA de Lyon in 2020. Her Ph.D. work on the fundamental combustion characteristics and chemistry of ammonia blend fuels was done under the joint supervision of Professor Hideaki Kobayashi at Tohoku University and Professor Dany Escudie at INSA de Lyon. Dr. Colson is currently working as a specially appointed assistant professor in the Institute of Fluid Science at Tohoku University. Her research focuses on the fundamentals of ammonia combustion for its use in industrial applications, including stabilization and emissions for both gaseous and liquid ammonia.

Abstracts

1. Data-driven prediction of flame lift-off-length and ignition delay of ECN spray-A

Balaji Mohan, Jihad Badra

Saudi Aramco, Saudi Arabia

Flame lift-off length (FLOL) and ignition delay time (IDT) are essential parameters in defining spray combustion characteristics. They help in understanding the combustion dynamics and validating the spray and combustion models for numerical simulations. However, obtaining extensive data from experiments is both a costlier and time-consuming task. As advancements in machine learning (ML) progress, ML could be used to build efficient models to serve as surrogates to experiments. Five different ML models have been trained in this study using the experimental dataset available through the engine combustion network (ECN) community. A novel genetic algorithm-based hyperparameter optimization code has been used to optimize the models to improve prediction accuracy. The model performances were compared, and the better model was chosen as an experimental surrogate to predict FLOL and IDT. Later the model predictions were compared with the experimental data.

2. A transfer learning approach to multi-target temperature-dependent reaction rate prediction

Emad Al Ibrahim, Aamir Farooq

King Abdullah University of Science and Technology, Saudi Arabia

The accurate prediction of temperature-dependent reaction rate constants of organic compounds is of great importance to both the atmospheric chemistry and combustion communities. Extensive work has been done on developing automated mechanism generation systems but the lack of quality data remains a huge bottleneck in the application of highly detailed mechanisms. Machine learning prediction models have been recently adopted to alleviate the data gap in thermochemistry and have great potential to do the same for kinetic data with the recent release of quality data compilations. The ultimate goal is to formulate easily accessible, general-purpose, temperature-dependent, and multi-target models for reaction rate data. To that end, we propose models that depend on the well-known Morgan fingerprints as well as learned representations transfered from the QM9 dataset. We propose the use of an Arrhenius based loss where predictions of the modified three parameters (A,n, and B=E_a/R) are given instead of the direct prediction of reaction rate constants.

3. Fuel Design using Genetic Algorithm and Artificial Neural Networks

Faisal Albaqami, Abdul Gani Abdul Jameel

King Fahd university of petroleum and minerals, Chemical Engineering Department, Dhahran, Saudi Arabia

Vincent Van Oudenhoven

Delft University of Technology, Mathematics and Computer Science Department, Delft, Netherland

The advancement during the era of the fourth industrial revolution lies in minimizing or eliminating human interference. This broadly applicable concept has found its course into the oil and gas sector. Pursuing opportunities in this sector has led to the identification of an auspicious application in fuel blending, an essential stage in refineries. At this stage, multiple streams are mixed to achieve the mandated fuel properties based on international and domestic standards. One of the mandated properties is Octane Number (ON). There are two forms of measuring ON: Research Octane Number (RON), and Motor Octane Number (MON). Although there were efforts in optimizing the blending operation, nonetheless, the implementation of machine learning models was limited. The intention behind exploring and enhancing this field is to avoid undesirable scenarios, such as off-specification products and quality giveaway, which overburden refineries' operational expenditures. This research presents an innovative approach to predict the optimum fuel blending mechanism. This is accomplished through utilizing an integrated system composed of a genetic algorithm (GA) and an artificial neural network (ANN). The system is highly capable of analyzing fuel input of pure hydrocarbons, hydrocarbon−ethanol blends, and FACE (fuels for advanced combustion engines) gasoline−ethanol blends. These fuel mixtures are presented as multiple input streams to the blending stage, at which the system computes different mixing scenarios utilizing the GA. Each scenario's dataset is converted to another set that is comprehended by the ANN model. The fuel input to the ANN model includes functional groups, branching index (BI) and molecular weight (MW). The functional groups include paraffinic CH3 groups, paraffinic CH2 groups, paraffinic CH groups, olefinic −CH=CH2 groups, naphthenic CH−CH2 groups, aromatic C−CH groups, and ethanolic OH groups. The integrated system was validated using 123 hydrocarbon-ethanol blends and 30 FACE gasoline-ethanol blends. The system is shown satisfactory results as its accuracy was compared against predicted RON, MON, and blends composition. The system resulted in R2 of 0.99 for both RON and MON. For the blend compositions, each component was evaluated independently with a total of thirteen components. The R2 value for these data ranged between 0.74 and 0.99. These results signify the success of the integrated system and its major potential impact in mitigating undesirable blending scenarios.

4. Machine Learning Model for Gasoline Compression Ignition at Low Loads

Zahra Al Ibrahim, Abdullah AlRamadan, Balagi Mohan, Jihad Badra

Saudi Aramco, Saudi Arabia

The study showcases the strength of machine learning (ML) models in imitating the operation of an advanced engine concept - the gasoline compression ignition (GCI) - at low loads. The ML models are trained on GCI engine experiments, covering different intake conditions, injection strategies and spark settings. The models have the capability to predict seven engine performance parameters: fuel consumption, four engine-out emissions, exhaust temperature, and coefficient of variation (CoV) in indicated mean effective pressure. Gradient boosting tree-based CatBoost regressors are the building blocks of the developed models. To obtain the most representative results of the model's accuracy, the models were evaluated using leave-one-out-cross-validation method. This paper shows that the seven models have successfully captured the complex

relationship between the input calibration parameters and the seven desired outputs. The developed models have the potential to be utilized in optimizing GCI engine performance - especially at low loads where the engine has issues lighting off the catalyst. Coupling ML models with suitable optimization algorithms can

pave the way to pinpoint the global optimum operation point in less time, and with less cost than traditional calibration approaches.

5. A machine learning surrogate approach for the optimization of fuel-engine design

Mohammed Almomtan, Aamir Farooq

King Abdullah University of Science and Technology, Saudi Arabia

Balaji Mohan, Jihad Badra

Saudi Aramco, Saudi Arabia

Optimization of internal combustion (IC) engines is a challenging task due to their highly nonlinear behavior and their associated expense of numerical simulation or experimental prototyping. Utilization of surrogate models as objective functions in the optimization task has proven to be an effective approach to reduce computational cost and overall runtime. However, appropriate selection of surrogate models remains to be a major challenge that is critical to both the accuracy of the obtained optimum and the total computational cost required.

In this work, an Artificial Neural Network (ANN) based surrogate was developed for the purpose of optimizing performance of IC engines. Tailored strategies for dealing with limited datasets were investigated to improve prediction accuracy and overall computational efficiency. Detailed descriptions of implemented strategies, including unsupervised pre-training and ensemble learning, are provided here. The developed surrogate was benchmarked to an ensemble Machine Learning (ML) model, known as SuperLearner, which is commonly used as a surrogate in recent IC engine optimization studies in literature. The developed ANN surrogate achieved higher prediction accuracy and better robustness compared to both SuperLearner and a standard ANN.

The ANN based surrogate shown here allows for the gradient of the target output with respect to model input parameters to be analytically calculated. This feature of the surrogate model is advantageous in that it permits the efficient utilization of Stochastic Gradient Descent (SGD) techniques to resolve the optimization task as opposed to the more commonly used and less computationally efficient heuristic approaches. An extensive analysis of the computational cost required for building the ML surrogate and resolving the optimization scheme for an engine optimization case study is performed here. The framework developed in this work proved to be significantly more efficient than heuristic-optimization based approaches.

6. Utilization of machine learning to predict the products' yields from co-pyrolysis of biomass and polymers

Aessa Alabdrabalnabi, Ribhu Gautam, Mani Sarathy

King Abdullah University of Science and Technology, Saudi Arabia

Biomass is an abundant and reliable energy source and chemical feedstock with 220 billion dry tons available globally. Thermochemical conversion of biomass can be used to mitigate the generation of 275 million tonnes of plastic waste. Biomass pyrolysis yields a low-quality pyrolytic oil due to its high oxygen content, pH, acidity, and viscosity. The pyrolysis bio-oil needs to be upgraded before being directly used as drop-in fuel and fuel additive. This upgrade can be achieved by co-pyrolysis of biomass with waste polymers. As polymers are a rich source of hydrogen, the pyrolysis vapors are upgraded by hydrodeoxygenation and hydrogenation reactions. The advantage of co-pyrolysis is that need for a separate hydroprocessing unit can be eliminated after adequate process optimization. Machine learning is emerging to be a growing field to predict and optimize energy-related processes. In this research, machine learning models were developed to predict the product yields from the co-pyrolysis of biomass and polymer. Data in the literature on the co-pyrolysis of lignocellulosic biomass and polymer co-pyrolysis was utilized to provide a tool to predict these reactor products. Classical machine learning and neural network algorithms were examined and trained with datasets acquired for biochar and pyrolytic liquid yields with cross-validation and hyperparameters to fit the ultimate and proximate analysis of the reactants and physical conditions of the reactions. The machine learning models provide a convenient predictive tool for co-pyrolysis reaction within the models' errors and training features' range. These models provide insights into the development of the thermochemical conversion of municipal solid waste in a circular carbon economy.

7. Large eddy simulation with flamelet progress variable approach via neural network acceleration

Lorenzo Angelilli, , Francisco Hernandez Perez, Hong Im

King Abdullah University of Science and Technology, Saudi Arabia

, Pietro Paolo Ciottoli, Mauro Valorani

Sapienza University of Rome, Italy

Despite recent advances in high-performance computing technology, detailed simulations of turbulent reacting flows remain challenging owing to the large number of equations associated with conservation of mass, momentum, energy, and chemical species concentrations, as well as the wide spectrum of spatial and time scales that are present in the system. Among reduced-order methods, large eddy simulation (LES) for turbulent flows and flamelet-based models for chemically reacting systems have gained widespread since they enable computations of reacting flows in an economic fashion while capturing key unsteady features of such flows.

In the flamelet-based models, chemical and thermochemical quantities are tabulated based on the solution of canonical laminar flames, which are expressed as a function of variables such as the mixture fraction and/or progress variable. To account for phenomena such as heat loss, pressure variations, and mixture inhomogeneities, additional variables must be included, increasing not only the dimensionality and storage requirements considerably, but also the computational cost associated with the look-up procedure.

Since the increase of dimensionality limits the applicability and expansion of tabulated combustion models, deep learning methods are an excellent candidate to substitute the well-established look-up techniques requiring large memory and multi-dimensional interpolation subroutines, often being memory intensive and not suited for modern CPU architectures.

In the context of LES of turbulent combustion, the flamelet/progress variable (FPV) model is widely employed and further considered here.

Recently, a neural network-based FPV was tested in a LES computation of the Sydney/Sandia flame. This work presents the approach employed to train an artificial neural network (ANN) on the flamelet/progress variable tables based on the mixture fraction, variance of the mixture fraction and progress variable. The training tables generated for a LES prediction of the hot coflow-piloted methane/air Sandia D jet flame are obtained by the solution of the steady laminar flamelet, and the so-obtained response surfaces are interfaced with the OpenFOAM solver. Their computational performance is assessed in a set of prototypical laminar computations in terms of absolute computational load and strong-scaling characteristics and accuracy in the prediction. A preliminary turbulent 3D comparison of the Sandia flame D is also presented.

8. The Future of Direct Air Capture at NEOM

Yasmeen Najm, Mani Sarathy, Roland Kaeppner

NEOM, Saudi Arabia

Greenhouse gas emissions have risen rapidly in the past 150 years with global temperatures 1.5C above pre-industrial era. Such increases lead to disruptions in the earth ecosystem with sea levels estimated to rise 0.6-1.6m by 2100 and higher frequencies in natural disasters. Current industrial emissions practices are unsustainable; bending the curve will require a coordinated global effort. Decarbonization will grow in urgency since efforts in emission reductions will not be enough to lower the 1.5C pathway. Direct air capture (DAC) is one solution to remove CO2 from the atmosphere at scale. NEOM's long term strategy and vision is capturing emissions from air, regardless of the source as a tool to reverse CO2 releases and utilizing the captured CO2 to create clean carbon neutral transport fuels such as green gasoline instead of storing CO2 underground. Currently, NEOM is building the largest green hydrogen plant at zero-carbon emission using renewable energy and desalinated water. Hydrogen is a unique vector to carry renewable energy beyond power lines but can also be combined with captured CO2 to create methanol via a hydrolysis process. Differing from hydrogen, methanol can be distributed and transported through existing gasoline infrastructure and pipelines. NEOM is uniquely positioned to pioneer in DAC with the ambition to tackle this generation's most pressing issue, its access to low-cost renewable energy which is highly competitive at lowest cost electricity (below 2 $/kwH) due to its unique solar and wind profiles, ample physical space to capture and store carbon, and highly supportive regulatory incentives for sustainability. Neom will build capabilities to incentivize long-term sustainability of DAC as it holds significant potential but will require 4 key unlocks to scale up within NEOM. Firstly, developments in technology with rapid cost-reduction through learning curve and standardization effects and deployment near low-cost renewable power sources by investing in R&D. Secondly, carbon revenue generation by finding mechanisms to monetize the captured CO2 to expand or enhance current business cases through pilot facilities. Thirdly, exploring for investors and project developers willing to take the risk to develop and scale emerging technologies that may completely or partially depend on regulations. NEOM will create coalitions of investors and project developers willing to take the risk to develop and scale emerging technologies Finally, obtain additional regulatory tailwinds to support CO2 capture technologies (e.g. tax incentives, ETS).

9. Analysis of methane, propane, and syngas oxy-flames in a fuel-flex gas turbine combustor for carbon capture

Medhat Nemitallah, Ahmed Abdelhafez

King Fahad University of petroleum and Minerals, Saudi Arabia

Premixed oxy-fuel combustion flames of methane, syngas (CH4:CO:H2 with the molar ratio of 2:1:1), and propane in CO2 diluted environment (for carbon capture) are examined in a swirl-stabilized gas turbine combustor using large eddy simulations (LES) in the full three-dimensional (3-D) domain. The flame and emission characteristics are examined for the different fuels over a range of equivalence ratio (Φ: 0.34, 0.39, and 0.42), at a fixed oxygen fraction (OF) of 60% (by volume), at fixed bulk inlet velocity of 5.2 m/s, and under atmospheric conditions. The results indicate increments in several characteristic parameters including adiabatic flame temperature (Tad), laminar flame speed (LFS), power density (PD), product formation rate (PFR), Damkohler number (Da), and CO emission, with the increase of Φ whatever the type of fuel. Alternatively, flame thickness (δ) decreases with the increase in Φ for the three fuels. Characteristic 'V' shape with almost identical outer recirculation zone (ORZ) is also observed for the three fuels. Among the studied fuels, oxy-methane flames demonstrate highest flame thicknesses, least uniform temperature distribution (highest pattern factor) at combustor outlet, and lowest CO emission level. Oxy-syngas flames show more uniform temperature distribution (lowest pattern factor) at combustor outlet and highest CO emission as compares to the oxy-methane and oxy-propane flames. The oxy-propane flames have higher values of Tad, LFS, PD, PFR, Da, and thermal power (TP) along with lowest flame thickness compared to methane and syngas counterparts.

10. Mobile Carbon Capture for Marine applications: An MDEA/PZ solvent process model case scenario

Fethi Khaled

Saudi Aramco, Saudi Arabia

Greenhouse gas (GHG) emissions, including Carbon Dioxide (CO2), are becoming a central challenge for the energy sector due to their role in climate change. Carbon capture is one of the many suggested solutions that could significantly reduce the carbon intensity of the fossil fuels. For instance, CO2 capture from stationary applications, such as power plants and refineries, has been applied worldwide for decades where the captured CO2 is sequestered for enhanced oil recovery (EOR).

The transport sector — which primarily involves road, rail, air and marine transportation — accounted for over 24% of global CO2 emissions in 2016 [World Resources Institute]. Mobile Carbon Capture (MCC) could be a plausible solution to reduce the carbon footprint of the transport sector and enable it to address the emission challenges established by the Paris Agreement.

This work will briefly discuss the various technologies used for carbon capture including chemical solvents, physical solvents, membranes and cryogenic separation and the challenges that are specific to on-board applications. A case scenario for mobile carbon capture on-board of a generic marine tanker using methyldiethanolamine/piperazine (MDEA/PZ) chemical solvent will be presented. We will also show the importance of exhaust heat recovery to decrease the energy intensity of the CO2 capture process and reach the high levels of CO2 avoidance that could enable the CO2 footprint targets of the International Maritime Organization (IMO).

11. Doping effect of oxygenated and non-oxygenated bio-oils on non-premixed turbulent hydrogen-based flames

Yilong Yin, Adam Gee, Kae Ken Foo

University of Adelaide, Australia

Bassam Dally

King Abdullah University of Science and Technology, Australia

Hydrogen has potential to be used as a renewable fuel in high-temperature industrial processes to mitigate CO2 emissions, by taking advantage of its carbon-free nature. One of the challenges to hydrogen application in industry is that hydrogen flames may have extremely low radiation, but such combustion systems typically rely on radiative heat transfer. Doping hydrogen with lignocellulosic biomass-derived bio-oils with high sooting propensity could be a promising approach to enhance the radiant intensity of hydrogen flames by promoting soot formation. In this study, the doping effect of bio-oils on flame structure, radiant intensity, soot formation and centreline flame temperature is measured using a combination of techniques including: still photographs, heat flux sensor, laser-induced incandescence (LII), and thermocouples. Due to the complex composition of bio-oils, toluene and anisole are selected as non-oxygenated and oxygenated bio-oil surrogates to emulate the chemical, physical and combustion properties of bio-oils for a lab-scale experimental study. Toluene is a prominent component of bio-oil and represents its aromatic structure with a methyl group attached. Anisole is an organic compound consisting of a phenyl group attached to a methoxy group which is the characteristic of a lignin structure. Non-premixed turbulent hydrogen-nitrogen (9:1 vol) flames are doped with 0.2 mol%, 0.3 mol% and 1 mol% (based on the molar concentration of hydrogen) prevapourised toluene and anisole. Toluene concentration has been further investigated at 3 mol% and 3.5 mol%. The results show that adding 0.2 mol%, 0.3 mol% and 1 mol% of dopant to the hydrogen-based flame has a slight non-linear positive impact on the radiant intensity and the signal of the soot formed in the flame is below the detectable level of LII at these dopant concentrations. The radiation enhancement becomes more evident when increasing the toluene concentration to 3 mol% and 3.5 mol%. Toluene, as a non-oxygenated dopant, is found to be more effective than anisole as a non-oxygenated dopant on radiation enhancement. The radiant intensity and soot formation tended to be more significant downstream of the flame. There is a marked centreline flame temperature drop observed downstream of the flame for high toluene concentration flame cases. This may result from the increased radiative heat transfer from the promoted soot formation.

12. A decoupling model approach to studying the pyrolysis and oxidation of C6-C10 saturated fatty acid methyl esters (FAMEs)

Xiaoyuan Zhang, Mani Sarathy,

King Abdullah University of Science and Technology, Saudi Arabia

Wei Li, Yi Zhang, Yuyang Li

Shanghai Jiao Tong University, China

Qiang Xu, Yixuan Jing Zhandong Wang

University of Science and Technology, China

Biodiesels are promising fuels for the transition to carbon neutrality. In terms of the molecular size and complex composition in real biodiesel fuels, it is a great challenge to develop compact enough kinetic models for practical purposes. The FGMech approach is proposed by this group for modeling real-fuel combustion based on constructing the intrinsic relationship between fuel structures and model parameters. It requires a database consisting of the model parameters for pure fuels. In this work, we selected five fatty acid methyl esters (FAMEs) as target fuels, including methyl pentanoate (MPE), methyl hexanoate (MHX), methyl heptanoate (MHP), methyl octanoate (MO) and methyl nonanoate (MN). Followed by the FGMech formulation, a decoupling model approach is adopted for model construction. Lumped reaction mechanisms are developed to describe the (oxidative) pyrolysis of fuels while a detailed model is used for describing the conversion of pyrolysis intermediates. To validate the present model, pyrolysis experiments for these FAMEs are conducted in a jet-stirred reactor (JSR) at 1 atm and over 790-1120 K. Both the synchrotron vacuum ultraviolet photoionization mass spectrometry (SVUV-PIMS) and gas chromatography (GC)/GC-MS are applied for measuring the pyrolysis intermediates. The fuels, primary hydrocarbon and oxygenated products, secondary products including various aromatic compounds, are identified and quantified for model validation. The present model can well-predict the temperature windows of fuel decomposition and reasonably predict the yields of most pyrolysis products against the present atmospheric pressure experimental data, as well as previous high-pressure pyrolysis data. The agreements between the measured and predicted results indicate that the present decoupling methodology can accurately describe the fuel decomposition and the evolution of intermediates under pyrolysis conditions. Besides, it is found that the increasing alkyl CH2 group from C6 to C10 FAMEs has little influence on the yields of primary oxygenated products, while leads to the increasing yields of hydrocarbon products, indicating that alkane chemistry becomes more and more important from MPE to MN. The present model is also validated against the high-temperature oxidation experimental data available in literature. Good agreements are observed between the measurements and the predictions.

13. Effect of Exhaust Gas Recirculation (EGR) and Ethanol Addition on Ignition Delay Times of Gasoline Fuels

Khaled Aljohani, Mani Sarathy, Aamir Farooq

King Abdullah University of Science and Technology, Saudi Arabia

Abd EI-Sabor Mohamed, Lu Haitao, Henry Curran

National University of Ireland, Ireland

The use of computational models are becoming significant path and analysis tool in the field of science and combustion. The prediction of real fuels behavior is the current motivation driving the kinetic modeling research. Nevertheless, understanding the reactivity of real gasoline fuels with exhaust gas recirculation (EGR) as well as ethanol additions in combustion environments remains incomplete. This work explores the reactivity behavior of two oxygenated gasoline fuels (Euro 6 and U.S Tier 3) and the variation of fuel reactivity with molecular composition. Furthermore, ignition delay times of Gasoline Euro 6 blended with exhaust gas recirculation (EGR) including NOx as well as Gasoline Euro 6/ethanol blends are provided in this work. The oxidation of the above-mentioned fuels have been measured in a high-pressure shock tube and in a rapid compression machine at two pressures of 20 and 40 bar, at equivalence ratios of ϕ= 0.50, and 1, and in the temperature range of 625-1420 K. Present work can provide valuable kinetic data to improve the current gasoline mechanisms as well as to include the NOx sensitization effect on real gasoline fuels.

14. High-Temperature Mid-IR Absorption and Kinetic Study of the Dioxolanes

Mohammed Adil, binod Raj Giri, Aamir Farooq

King Abdullah University of Science and Technology, Saudi Arabia

Milán Szőri, Lam K. Huynh,

University of Miskolc, Hungary

Cyclic saturated ethers can be promising bio-derived fuel for future sustainability. Despite, the pyrolysis and combustion behavior of these fuels are not well understood. Among the saturated cyclic ethers, dioxolanes have been identified as a promising biofuel. Aiming to characterize the combustion behavior of dioxolanes, we have carried out the temperature-dependent absorption cross-section between 950-1190 cm-1 and apply the spectroscopic knowledge to rationalize the temperature and pressure dependence of the rate coefficients for the unimolecular decomposition of 1,3-dioxolanes (13DO) and 2-methyl-1,3-dioxolanes (2M13DO). We employed a rapid tuning MIRcat-QTTM laser that can be operated either at a fixed wavelength or over a wide range of wavelength (845 cm-1 - 1470 cm-1). We used MIRcat-QTTM laser in conjugation with a shock tube to carry out the high temperature spectroscopic and pyrolysis measurements near 1 bar. The measured IR absorption spectra are the first collection of high-temperature spectra of these species, which exhibit strong temperature dependence. In addition, we employed the composite quantum chemical method (W1U) to explore the potential energy profiles of the possible unimolecular decomposition pathways of 13DO and 2M13DO. We obtained the phenomenological rate coefficients, k(T, P), and time-resolved species profiles using the stochastic RRKM-ME model. Our theoretical model accurately captured the experimental trends of the rate coefficients for the unimolecular decomposition of 13DO and 2M13DO.

15. Minimum ignition energy measurement of methane-air at cryogenic conditions

Anupam Ghosh, Deanna Lacoste

King Abdullah University of Science and Technology, Saudi Arabia

The main objective of this study is to investigate the minimum ignition energy (MIE) of premixed methane-air under cryogenic conditions (< 273-K). There is a dearth of data on the minimum ignition energy and the flame speed of premixed methane-air and hydrogen-air at cryogenic conditions. This unexplored area motivated us to explore through this current study. Studies in the literature have reported that initial mixture temperature considerably affects the minimum ignition energy. Thus, it is essential to understand the effect of lower initial temperature on the minimum ignition energy, which plays an important role in air-fuel ignition. The impact of low temperature on minimum ignition energy is studied for various initial temperatures of the methane-air mixture. Liquid nitrogen was used to create lower methane-air mixture temperatures ranging from 200-K to 273-K. Experiments were conducted at atmospheric pressure using a Bunsen burner by keeping the equivalence ratio constant at 1. An electrode with a gap distance of 1-mm and a pulse of 100-μs duration were incorporated to ignite air-fuel mixtures. The data on minimum ignition energy of premixed methane-air at atmospheric conditions are compared with those of existing data from the literature to validate the results from the current experiments. The data from this current study will serve as a valuable benchmark for validating computational models of the minimum ignition energy and the flame speed at cryogenic conditions. Overall, this work has yielded beneficial results and guidelines regarding safety requirements for fuels such as methane and hydrogen during storage at low temperatures.

16. Direct numerical simulations of super-knock development process in IC-engine conditions

Minh Bau Luong, Hong Im

King Abdullah University of Science and Technology, Saudi Arabia

Super-knock is a developing detonation process characterized by excessive pressure oscillations and extremely high-pressure spikes that can damage combustion-chamber components. The fundamental understanding of the developing super-knock mechanism and a reliable criterion to predict it are needed to prevent destructive operation of combustion devices. As such, direct numerical simulations (DNS) are performed in this study to unravel the underlying mechanism of the onset of super-knock development in realistic internal combustion (IC) engine conditions. Motored-pressure and motored-temperature history profiles under realistic IC engine conditions are reproduced by applying a compression heating model. Dimethyl ether (DME) exhibiting a representative two-stage ignition process, and a strong negative temperature coefficient (NTC) behavior is adopted as a fuel. A set of parametric simulations is performed by varying the initial mean temperatures lying in three different low-, intermediate- and high-temperature regimes, and the temperature fluctuation level, under two different intake pressure. We found that the strong heat release rate from the first-stage ignition enhances the propensity of super-knock development. Particularly, it has a pronounced effect in reducing the minimum characteristic length scale requirement of temperature field to form detonation waves. The theoretical analysis is conducted and reveals that the minimum running distance allowing detonation formation in the low-temperature regime is within the same order of magnitude with that in the intermediate- and high-temperature regime. Consistent with the theoretical analysis, the DNS results verify that at the same characteristic length scale of temperature field, the low-temperature cases are also able to form detonation waves, leading to excessive pressure oscillations and extremely high-pressure spikes.

17. Numerical study on NOx formation in premixed turbulent C3H8-air flames diluted with CO2-H2O

Abdelkader Hemaizia, Abdelhalim Bentebbiche

University of Sciences and Technology Houari Boumediene, Algeria

The addition of the exhaust gas with reactant mixture is well known technique used for reducing NOx emissions in gas turbine combustor, and this effective technique is receiving more attention in the last decade because of its positive effect on pollutant emissions. This paper investigates the thermal effect of CO2+H2O dilution ratio on the global NOx formation rate in premixed turbulent C3H8-air flames in a swirled burner at atmospheric pressure. The numerical study is performed using commercial CFD code fluent (2019). All simulation cases are based on reynolds average navier stokes formulation, and the standard k-ε model is adopted as a turbulent closure. The turbulence-chemistry interaction (TCI) is modeled using finite rate-eddy dissipation model (FR/EDM). Three-step reaction mechanism is adopted in this study.The study is conducted using only one volumetric fraction with three combination of CO2+H2O, XCO2+H2O = 16% (12% CO2+4% H2O; 8% CO2+8% H2O; 10% CO2+6% H2O; 6% CO2+10% H2O), two Reynolds number, Re = 39 ×104, Re = 29 ×104, swirl number Sn = 0.6 and equivalence ratio of 0.8. The flame shape, Combustor temperature, and the NOx and CO concentration is depending on these parameters. Result show that the flame temperature and its length, NOx and CO emissions decrease drastically with the addition of CO2 and H2O. Various combinations of CO2 and H2O decreases the flame temperature but create a fluctuation on its values that confined between 1798 K and 1849 K. This makes the NOx and CO concentration at the combustor outlet change irregularly depending on the mixture composition. The formation of NOx emissions is sensitive to the flame temperature where its values vary from 0.27 ppm to 0.7 ppm, as well as the CO concentration from 33 ppm to 65 ppm, respectively.

18. Autoignition Experiments of Iso-octane at Ultra-Lean and Lean Conditions

Khayyom Hakimov, Yang LI, Mani Sarathy, Aamir Farooq

King Abdullah University of Science and Technology, Saudi Arabia

Yang LI

Northwestern Polytechnical University, Xi'an, China

Ignition delay times (IDTs) of iso-octane were measured in a high pressure shock tube and a rapid compression machine at ultra-lean to lean equivalence ratios (Φ = 0.2 - 0.6) relevant for Pre-Chamber Combustion (PCC) systems. Measured IDTs were longer for lower equivalence ratios and lower pressures. The equivalence ratio effect was more prominent in the intermediate temperature range. The existing models from the literature showed notable differences with newly obtained data at fuel-lean conditions. Temperature and OH sensitivity analyses were performed to identify main reactions affecting the reactivity at different temperatures. Rate constants of two key reactions were modified to improve model performance at intermediate and low temperature ranges.

19. Numerical study of lean premixed humidified hydrogen-methane-air combustion in a generic triple swirl burner

Neha Vishnoi, Lipika Kabiraj

Indian Institute of Technology Ropar, Punjab, India

Agustin Valera Medina

Cardiff University, Wales, United Kingdom

Aditya Saurabh

Indian Institute of Technology Kanpur, Uttar Pradesh, India

Increasing energy demand, limited non-renewable resources, a requirement for increased operational flexibility, and the need to reduce pollutant emissions are the critical factors that drive the development of next-generation fuel-flexible gas turbine combustors. The use of hydrogen and hydrogen-rich fuels such as syngas helps in achieving decarbonisation. However, high temperatures associated with hydrogen increases NOx emissions. Humidified combustion presents a promising approach for NOx control. Humidification reduces the flame temperature, and, therefore, restrains the thermal NOx formation pathway (Göke et al., AIAA, p.1272, 2012). The challenge in the implementation of the humidified combustion is the combustor that must maintain a stable flame with low emissions up to very high degrees of water or steam dilution. Additionally, the combustor (burner) should have high fuel flexibility and enable operation on natural gas, syngas, and also pure hydrogen. In the present work, we investigate the flow fields and combustion characteristics of a generic triple swirl burner running on premixed humidified and hydrogen-enriched methane-air mixtures. The investigated burner consists of three co-axial co-rotating swirling passages: outer radial swirler stage and two inner concentric axial swirler stages. Reynolds Averaged Navier-Stokes (RANS) simulation approach describes the flow within the burner and inside the combustor. We investigate the flow fields, NOx emissions, flame behaviour and its stability against flashback for hydrogen-enriched methane-air mixtures based on the characterization of velocity profiles, streamwise and azimuthal shear layers, and temperature fields. We present the experimental validation of isothermal velocity profiles inside the combustor. We also investigate the effect of humidified combustion for methane-hydrogen blends and compare temperature estimations and NOx emissions.

20. Active Control of Thermoacoustic Instabilities in a Premixed Laminar Flame Using Time Phased Bursts of Nanosecond Repetitively Pulsed Discharges

Ammar Alkhalifa, Abdulrahman Alsalem, Davide Del Cont-Bernard, Deanna Lacoste

King Abdullah University of Science and Technology, Saudi Arabia

Thermoacoustic instabilities are a type of combustion instability where the interaction of heat release of combustion and the natural acoustics of the system cause the combustion to be unstable. Thermoacoustic instabilities can damage combustion systems due to unstable heat release and strong pressure fluctuations. Various plasma discharges have been shown to suppress thermoacoustic instabilities in the literature. Non-equilibrium glow plasma can be produced with Nanosecond Repetitively Pulsed (NRP) discharges with a relatively low energy deposition. In this project, the use of NRP discharges to suppress thermoacoustic instabilities in an axisymmetric wall-stabilized premixed laminar methane/air flame is investigated. An active control scheme is implemented where the pressure waves produced by an unstable flame are measured and in-phase bursts (90, 75, 60, or 45 pulses for each burst) of NRP discharges are sent to suppress the instability. A parametric study was done to investigate the effect of discharge voltage, NRP discharge frequency, discharge burst phase shift, and discharge burst frequency on suppressing the thermoacoustic instability. The control scheme can either have no measurable effect or a significant effect on suppressing the thermoacoustic instability depending on the scheme's parameters.

21. Fuel economy assessment of modern engine technologies in a range-extended electric vehicle

Emre Senker
Saudi Aramco, Saudi Arabia

Vehicle simulations have been performed to assess the fuel consumption of a compact class range-extended electric vehicle equipped with four different novel engines in addition to the baseline production engine. These new engines are currently in development phase and the analysis in this work is done based on their laboratory measurements. Each of these engines has a unique component technology for reduced emissions: the first engine employs a turbulent jet ignition system, the second engine works on an extreme Miller cycle, the third engine has a two-stroke opposed-piston architecture and the fourth one is a direct-injection hydrogen engine. The assessment was done over WLTC driving cycle that provides a balanced composition of urban and rural driving. The battery management system was set to charge sustaining mode to maintain the state of the charge around a fixed level throughout the driving cycle. All five engines were scaled to same maximum power to ensure a fair comparison. A comparison with original (unscaled) engine specifications was also included in this study. The simulations with gasoline engines showed that next engine technologies will provide up to 20% improvement of fuel economy with respect to the baseline engine. Hydrogen engine simulations showed that with its compact size and high-power density, it can be considered as a zero-tailpipe emission option as a range extender. The results of this work provide a database for estimation of the CO2 emissions of the passenger vehicles in the decades to come.

22. An unconventional internal combustion engine as a range extender for low carbon mobility

Giovanni Vorraro, James Turner
King Abdullah University of Science and Technology, Saudi Arabia

The automotive sector is facing an extraordinary time as a consequence of the several announcements, by different countries, regarding the future ban of the internal combustion engines in favour of the battery electric vehicles (BEVs). Although the BEVs, with their zero tailpipe emissions, represent a valid solution in countries producing electricity from renewable sources, a series hybrid powertrain (or range-extended electric vehicle, REEV) layout, based on a small internal combustion engine used as a range extender and an electric motor for the vehicle traction, is representative of an optimal solution where charging infrastructures are not developed yet or the production of electricity is still based on coal.

In that respect, an interesting engine architecture for range extender application is represented by the rotary Wankel engine. With its extraordinarily favourable power-to-weight ratio and high power density in addition to a compact design with low vibrations, the rotary engine has the potentiality as the ideal range extender, especially when fuelled with alternative fuels as the Hydrogen.

This work will present the experimental activities on the 225CS rotary Wankel engine (225cm3) produced by Advanced Innovative Engineering UK (AIE UK). Specifically, it will illustrate the particular combustion analyser developed to collect the indicated pressure cycles together with the other experimental results regarding the performance and the emissions of the engine fuelled with conventional fuel. Relying on those data, further considerations will be made on the development of a dedicated injection system in order to run the engine on Hydrogen fuel, while performance predictions using the alternative fuel will be made by modelling activities. Finally, the numerical results will represent the baseline for a future development strategy able to reduce the carbon footprint of the rotary engine applied as a range extender.

23. Ignition regimes of GCI engines and the usefulness of autoignition surrogates for GCI fuels with varying sensitivities

Jihad Badra, Fethi Khaled, Tamour Javed

Saudi Aramco, Saudi Arabia

Aamir Farooq

King Abdullah University of Science and Technology, Saudi Arabia

Engine and spray simulations require the use of carefully designed surrogate fuels that mimic the properties of the real fuels. Generally, these surrogates range from simple primary reference fuels (PRFs) to complex multi-components mixtures. In this study, the surrogate requirements for gasoline compression ignition (GCI) engines are extensively investigated under various operating conditions covering the entire engine speed-load map. The boundary and initial conditions for eleven different speed-load points were obtained from experiments. The data covered engine loads between 1 and 22 bar indicated mean effective pressure (IMEP) and engine speeds between 800 and 2500 revolutions per minute (RPM). Two gasoline fuels with different sensitivities were investigated here. The first was a high sensitivity (S=11) certification gasoline (Haltermann CARB LEV III E10) with a research octane number (RON) of 91 and the second was a low sensitivity (S≈0) Fuels for Advanced Combustion Engine (FACE) gasoline with a RON of 84. Two multicomponent surrogates (up to 8 components) were used as baselines for the chemical kinetic simulations of the two respective gasoline fuels. In addition, PRF, toluene PRF (TPRF), and ethanol TPRF (TPRFE) surrogates were thoroughly investigated at all speed-load conditions to determine the usefulness of these surrogates in the engine speed-load domain. Ignition kinetics were simulated using Chemkin-Pro software. Constant volume zero-dimensional (0D) and homogeneous charge compression ignition (HCCI) modules in Chemkin were used in this work. The simulations were analyzed using Livengood-Wu integral to determine the temperature range at which combustion occurs in GCI engines at different speed-load conditions. It was found that, except at the limiting high-load conditions, the temperature at ignition onset in a GCI engine is in the 850-950 K range. The low-temperature (<700 K) reactivity exhibited negligible contribution to the main ignition phenomenon. Two stage ignition and cool flame kinetics were found to dominate mid-load kinetics especially for the low-sensitivity fuel. Simple PRF surrogate was found to be sufficient to mimic the ignition requirement of the low-sensitivity gasoline fuel at almost the entire GCI engine speed-load regime. However, for the high-sensitivity gasoline fuel, it was found that PRFs are good surrogates only at high-load conditions where the in-cylinder pressures and temperatures are particularly high (>30 bar, >1100K). However, at low- and medium-load conditions, significant differences in the crank angle at 50% heat release (CA50) can be observed when using PRF to mimic the auto-ignition of high-sensitivity gasoline. In these regimes, TPRF and TPRFE surrogates show better representation of the auto-ignition behavior of the high-sensitivity fuel.

24. Numerical Evaluation of Cold Operation Strategies in a Heavy-Duty Gasoline Compression Ignition Engine

Emma Zhao, Yu Zhang, Yanjiang Pei, Anqi Zhang

Aramco Services Company, USA

Muhsin Ameen

Argonne National Laboratory, USA

Gasoline compression ignition (GCI) offers the potential to markedly improve the NOx-PM tradeoff over conventional diesel combustion while achieving high fuel efficiency. However, due to gasoline's low reactivity, it is challenging for GCI to attain robust ignition and stable combustion under cold operating conditions. In this work, 3D computational fluid dynamics (CFD) simulations were performed to understand and optimize GCI combustion under cold idle operating conditions. The CFD model validation was performed against GCI experimental results obtained from a 15 L heavy duty diesel engine operated at 17.3 compression ratio (CR) using a RON92 E0 gasoline. Building on the understanding acquired on the GCI spray, ignition and combustion processes, a numerically aided calibration investigation of varying cold start assistance strategies was conducted. The influence of each strategy on enhancing the GCI combustion process under cold operation was evaluated. The numerical analysis showed that using an intake air heater in the current engine was challenging to assist ignition at very low temperatures. Both glow plug and spark plug were effective in enhancing GCI combustion during cold operation but were sensitive to injector spray pattern and fuel injection strategies. These findings laid a solid foundation to guide hardware selection towards developing future near-zero emissions transport solutions.

25. A Computational Investigation of the Combustion Behavior and Turbulence-Chemistry Interaction in a Narrow-Throat Prechamber Combustion Engine

Mickael Silva, Xinlei Liu, Hong Im
King Abdullah University of Science and Technology, Saudi Arabia

Emre Cenker
Saudi Aramco, Saudi Arabia

Advanced modeling tools and techniques are essential for the development of high-efficiency engines with low CO2 footprint. Towards fundamental investigation of key physical aspects of prechamber combustion, the current work utilizes CONVERGE, a computational fluid dynamics solver, to understand the fundamental of turbulence chemistry interaction in a large bore engine operated with methane. The prechamber is composed of an upper conical part that lodges the spark plug and fuel injector, followed by a straight and skewed region called throat, which tip accommodates the nozzles responsible for the charge exchange between the prechamber and main chamber. The combustion is modeled with the G-Equation; the laminar flame speed was obtained from a lookup table generated from a methane oxidation mechanism reduced from the GRI 3.0, while the turbulent flame speed was computed using the well-known Peter's relation. Therefore, the turbulence-chemistry interaction is taken into account. A homogeneous charge of methane is considered at the intake port, maintaining the global $\lambda = 1.8$, with 3% of the total fuel being added through the prechamber. The results show that the flow field inside the prechamber and the jet generated by it are highly turbulent. This indeed governs critical aspects of initiation and maintenance of the combustion processes happening in the pre and main chambers. The combustion regime according to the Borghi diagram was found to lie initially in the thin reaction zone and lately in the corrugated flamelet regime.

26. A Priori Computational Assessment of Laminar Flame Speed Correlation in an Ultralean Prechamber Engine

Gufran Alkhamis, Mickael Silva, Hong Im

King Abdullah University of Science and Technology, Saudi Arabia

Emre Cenker
Saudi Aramco, Saudi Arabia

Gulder's correlation for the laminar burning velocity was investigated numerically and compared to engine experimental results from KAUST through computational fluid dynamics using CONVERGE. The ultimate goal is to adjust Gulder's empirical constants to satisfy lean-burn engine conditions. A discrepancy was numerically observed between the baseline case, which utilizes a tabulated laminar flame speed from the skeletal GRI3.0 by Lu and Law, and the results yielded by Gulder's relation. For both cases, Peter's turbulent flame speed correlation was utilized; therefore, any discrepancy, if present, should arise from the laminar flame speed. This modification aims to eliminate the need to refer to extensive chemical mechanisms or tabulated data and establish a simple and reliable model for the prediction of the laminar burning velocity at practical engine conditions. Gulder's correlation was adjusted by changing the values of its empirical constants α, η, and ξ to meet similar behavior encountered at high pressures and high temperatures when utilizing Lu and Law's mechanism. When implemented in CONVERGE, the updated Gulder's model can predict the KAUST experimental data which the original Gulder's model fails to match to.

27. Multiple injections to enable fuel flex engines

Bassam Aljohani, Ailobat, Aibolat Dyuisenakhmetov, Moez Ben Houidi, James Turner, William Roberts

King Abdullah University of Science and Technology, Saudi Arabia

A potential pathway to efficiency gain in a CI combustion is to avoid the limitation of, in cylinder high temperature, as it is a significant enabler to heat transfer losses and NOx/soot formation. This high temperature entails a diffusion-driven combustion with large burn rate. Isobaric combustion is proven to burn similar diffusion combustion but with a lower in cylinder temperature, in comparison to conventional diesel combustion (CDC) with comparable efficiency and emissions. In this study, fuels with high octane ratings are considered to provide further understanding on isobaric combustion utilizing Primary Reference Fuel (PRF) in a heavy duty CI engine of single injector setup, with multiple injection strategies. The fuel flow rate of each injection of a four injection strategy is reproduced and characterized by high pressure fuel pump test rig equipped with a piezoelectric pressure sensor to measure the spray momentum force. Measurement of injection rate and mass for each fuel also aids the development of isobaric combustion modeling. The study is focused to demonstrate the role of fuels on isobaric rate of heat release (RoHR) from low to high load conditions. With diesel fuel, isobaric combustion is initiated with the 1st injection irrespective of loads. In contrast, fuels like isooctane exhibit distinct start of ignition. At low loads, the 1st and 2nd injections are ignited by the 3rd injected spray with extended premixing process resulting in partial premixed combustion (PPC) at 50 bar. With 70 bar case, combustion is initiated by the 2nd spray while the 3rd and 4th injections are a typical diffusion combustion regime similar to CDC. Boosting toward intermediate loads, Isooctane has the advantage to advance start of injection to overcome the large burn rate associated with diesel. Diffusion controlled combustion is realized at high loads with ignition of the 1st injection. At high loads, the peak motored cylinder temperature and pressure are 950 K and 150 bar respectively which allow to phase combustion of isooctane with the 1st injection similar to diesel fuel at these conditions with improvement on NOx/soot emissions and comparable engine efficiency.

28. Enhancing Ammonia Combustion by Blending with Diethyl Ether

Binod Raj Giri, .Aymen Elbaz, Gani Issayev, William Roberts, Aamir Farooq

King Abdullah University for Science and Technology, Saudi Arabia

Krishna Prasad Shresth, Fabian Mauss

Brandenburg University of Technology, Germany

Lars Seidel

LOGE Deutschland GmbH, Germany

This work presents an experimental and kinetic modeling study characterizing the combustion behavior of ammonia blended with diethyl ether (DEE, 5-40% by mole). In this work, we employed a constant volume spherical vessel to measure the laminar flame speed of NH3-DEE blends at 298 K and elevated pressures of 3 and 5 bar, and equivalence ratio ranging from 0.8 to 1.3. We developed a detailed kinetic model to describe the experimental trends of the laminar flame speed and ignition delay times of NH3/DEE blends. The kinetic model was first validated against pure NH3 and DEE components experimental data from shock tube, plug flow, and jet-stirred reactors, freely propagating, and burner-stabilized premixed flames. Then it was validated by exploiting our earlier published ignition delay times data from a rapid compression machine over a temperature range of 620 to 942 K, pressures near 20 and 40 bar, equivalence ratio of 1 and 0.5. Overall, our kinetic model performed remarkably well to reproduce the experimental data for pure DEE, and NH3/DEE blends for a wide range of investigated conditions. The results show that DEE is very effective in enhancing the combustion characteristics of NH3. We found that the cross-reactions between the nitrogen and carbon family are critical to accurately predict the autoignition timing. This work will provide a detailed chemical insight into the interaction of NH3 and DEE sub-chemistry. The findings could be valuable to understand the oxidation kinetics of other nitrogen and carbon-based fuels. In our contribution, the combustion behavior of various NH3-DEE blends will be compared and discussed.

29. Experimental Rig for Hot Ammonia Nitridation Studies

Nocole Laws, Ziad Dawood, Saumitra Saxena, Sreenivasa Gubba, William Roberts

King Abdullah University for Science and Technology, Saudi Arabia

As the urgency for a carbon-neutral economy increases, finding suitable energy sources to meet the current demand is essential. Ammonia, NH3, has been proven to be a promising energy carrier and an excellent candidate for hydrogen extraction, making it a favorable contender in the future of sustainable energy.

Ammonia is incompatible with many industrial materials due to the adverse effects of both nitridation, an ingress of atomic nitrogen through the surface, and hydrogen embrittlement. The available information on the corrosive effect of NH3 on exposed materials at high pressures and temperatures for long durations is limited. In order to understand this effect, an experimental corrosion rig, originally designed for liquid fuel combustion to understand the hot corrosion mechanism of vanadium-sodium-sulfur-containing fuels on thermal barrier coatings (TBCs), at KAUST is currently being modified. This corrosion rig will be adapted to suit the current ammonia needs pertaining to high pressures, greater than 20 bar, and high temperatures, up to 850°C, for long operational hours.

The corrosion rig will house samples, varying in metallic and non-metallic nature, of coupons and coatings exposed to the parameters of interest. These samples will be further analyzed metallurgically to help provide insight into the nitridation and hydrogen embrittlement effect of materials during commercial applications of hot ammonia exposure. Learnings from various preliminary tests and rig modifications will be presented.

30. Oxidation of formic acid and decane using Jet Stirred Reactor

Shamjad Moosakutty, Mourad Younes, Mani Sarathy

King Abdullah University for Science and Technology, Saudi Arabia

The use of pure hydrogen as fuel creates significant logistical requirements and safety concerns. Therefore, identifying 'hydrogen carrier' compounds to store and transport hydrogen safely is of great interest. Formic acid has been gaining recognition as a hydrogen carrier molecule. Identifying the chemical kinetic pathways is necessary to form a kinetic model for formic acid. This study aims to provide experimental data to develop and validate kinetic models for the combustion of formic acid, decane, and its mixture. The experimental data is obtained by reacting the fuels in the presence of varying oxygen concentrations within a jet-stirred reactor (JSR).

The experiments were conducted individually on pure formic acid and decane first. The initial concentration of both fuels was set to 1000 ppm. Fuel was injected using a flow-controlled syringe pump. A vaporizer operating at 473 K was used to convert the liquid fuel into gas. The amount of oxygen reacted was varied depending on equivalence ratios (φ) of 0.5, 1.0, and 1.5. The residence time for gases within the JSR was set to be one second, and the temperatures were varied from 473 to 1000 K with a 50 K increment. The fuel and oxidizer were carried through the JSR system using nitrogen as a carrier gas. A Fourier transform infrared (FTIR) spectrometer mounted with a 2 m gas cell was used to measure the combustion emissions. For the study of fuel mixture containing formic acid and decane, a gas chromatograph (GC) with both FID and TCD detectors was used. The ratio between decane and formic acid was varied at 10, 30, and 50%. The equivalence ratios were kept at 0.5, 1.0, and 1.5.

During the pure form combustion experiments, the formic acid gets completely consumed around 950 K. The conversion of formic acid to CO and CO2 is most active between the temperatures 700-950 K. The decane concentration shows an initial decrease around 600 K, then increases to the original values until 800 K. The concentration decrease further and gets completely consumed around 1000 K for $\varphi = 0.5$. For $\varphi = 1$, the final temperature is 1100 K. The experimental values will be compared to existing kinetic models and be used for further improvements.

31. Hydrogen evolution from hydrocarbon pyrolysis in a simulated liquid metal bubble column reactor

Fabiyan Angikath Shamsudheen, Faseeh AbdulRahman, MuraliKrishna Khandavilli, Xiaoyuan Zhang, Mani Sarathy

King Abdullah University of Science and Technology, Saudi Arabia

The evolution of hydrogen from methane decomposition in a liquid metal bubble reactor (LMBR) has become a recent subject of interest; this study examines a novel approach to hydrogen production from pyrolysis of complex hydrocarbon fuels. Modeling hydrocarbon fuel decomposition in an LMBR is executed in two stages of pyrolysis: First, primary pyrolysis intermediates are simulated using a functional-group-based kinetic model (FGMech). Then, a detailed high temperature mechanism (AramcoMech 1.3 + KAUST PAH + 5 solid carbon chemistry) is applied to simulate secondary pyrolysis of intermediates. The quantities of major products of the secondary pyrolysis simulation (CH4, H2, Cs, C6H6) are approximated by simplified regression equations. Further decomposition of smaller hydrocarbons (until exiting the reactor) is simulated using a coupled kinetic and hydrodynamics model that has been reported in the literature. The mixing effects of bubble coalescence and breakup are investigated in a comparative study on homogeneous and non-homogeneous reactors. Finally, a qualitative relationship between H2 yield per mass of fuel, functional group, and other factors such as temperature, pressure, and residence time is analyzed. In general, the H/C ratio and cyclic/aromatic content are the main features influencing total conversion to H2.

32. DNS of hydrogen flames at elevated pressures: turbulent flame speed analysis

Wonsik Song, Francisco E. Hernández Pérez, Hong Im

King Abdullah University of Science and Technology, Saudi Arabia

To better understand the turbulence-flame interaction in practical combustion environments, lean hydrogen-air premixed flames are computationally investigated at elevated pressures up to 7 atm. High-fidelity direct numerical simulations (DNS) with detailed chemistry and transport are conducted using the recently developed simulation code called KARFS (KAUST Adaptive Reacting Flow Solver). Two sets of simulations are performed: Set1 corresponds to fixed velocity scale ratios (u'/SL = 3.0) and length scale ratios (Lt/df = 1.2) in the Borghi diagram, while Set2 corresponds to fixed velocity scale ratios (u'/SL = 3.0) and increasing length scale ratios (Lt/df = 1.2, 4.2, 7.0, 9.4), yet the physical integral length for the Set2 is identical. The ratio of turbulent flame speed to laminar flame speed is found to increase with the pressure for both sets. Statistical analysis of the flame curvature via the probability density function (PDF) reveals that the highest probability of the flame curvature is shifted from negative to positive as the pressure increases, leading to the local flame speed enhancement. For Set2, the increase in flame speed is mainly due to the flame surface area enhancement without any sharp increment of the turbulent flame speed, while for Set1 at high pressure (e.g., 7 atm), sharp increments in the turbulent flame speed are observed. Through statistical analysis of the local flame structure for selected peaks and valleys, this sharp increment in the turbulent flame speed is found to be related to the thermal-diffusive instability effects, yet the hydrodynamic instability effects are reduced. On the other hand, for Set2, the thermal-diffusive effects are less pronounced.

33. Hydrogen as a fuel for HCCI engines

Abdulrahman Mohammed, Inna Gorbatenko, Mani Sarathy

King Abdullah University of Science and Technology, Saudi Arabia

Hydrogen combustion in internal combustion engines is an attractive candidate for addressing climate change owing to its near-zero emissions. Hydrogen fuel has been studied in spark ignition (SI) engines and showed a high octane sensitivity, denoted as the difference between RON and MON. The only harmful emissions from hydrogen combustion in SI mode are nitrogen oxides as a result of high temperature nitrogen oxidation reactions. Homogeneous Charge Compression Ignition (HCCI) is a low temperature combustion technology that can potentially solve the problem of NOx emissions, at the same time achieving higher thermodynamic efficiency. Several studies have investigated the combustion of pure hydrogen in HCCI mode at different operating conditions. However, there has not been a comparison between hydrogen and reference hydrocarbon fuels, such as n-heptane and iso-octane. The present study focuses on evaluating the HCCI performance of hydrogen in the light of the Lund-Chevron HCCI fuel number. The experiments are conducted in a modified Cooperative Fuel Research (CFR) engine to run in HCCI conditions using hydrogen port injection. Here, the auto-ignition of hydrogen is compared to the auto-ignition of reference fuels at different engine speeds and intake temperatures. The results show that hydrogen HCCI combustion is sensitive to engine operating conditions with hydrogen behaving as a high octane fuel at low engine speeds and intake temperature, while low octane rating is encountered with increasing speed and intake temperature. The study also sheds light on the problems and drawbacks associated with hydrogen combustion in HCCI engines, as well as potential solutions to such problems.

34. Characterization of a novel dual-fuel, dual-swirl burner for carbon free fuels

Amit Katoch, Thibault F. Guiberti, Deanna Lacoste

Saudi Aramco, Saudi Arabia [1]

King Abdullah University of Science and Technology, Saudi Arabia

In recent years, the focus of the global energy generation (power and transportation) sector has shifted towards carbon-free fuels. In this context, hydrogen and hydrogen carriers have emerged as favorable candidates for this transition. Amongst the hydrogen-carriers, ammonia is much in the limelight due to its established methods for storage and existing infrastructure for supply and distribution. The present work is focused towards the development of a dual-fuel, dual-swirl burner where the combustion of hydrogen-ammonia mixtures would be studied in future. The preliminary steps of characterizing the newly designed burner were carried out. Methane-air mixtures were used to assess the capability of the burner to stabilize turbulent swirl flames at atmospheric pressure for a thermal power range of 5-8 kW. A 40° swirler was used along with different geometrical configurations to regulate the mixing of the two concentric fuel-air premix streams. The stability map indicates that, within the bounds of aforementioned thermal power, flames could be stabilized for a global equivalence ratio range of 0.64-0.72. V and M shape flames could also be observed which are typical of such burner configurations. The control of mixing between the two premix streams upstream of the injector resulted in different stability regimes. The central rod was seen to anchor the flame regardless of the extent of mixing upstream of the injector. For a fixed thermal power, the flame shape could be modulated by changing the internal geometry and swapping the two premix streams. Based on previous findings from the literature, this in turn indicated that the thermoacoustic response could also be tuned.

35. Challenges on the road to zero-emission vehicles

Fakhar Mahmood

Saudi Aramco, Saudi Arabia

The biggest challenge transport industry in particular and all energy sectors in general are facing today, is to reduce the GHG emissions towards a carbon-neutral mobility by 2050 and the reduction of pollutant emissions to meet air quality requirements. IC Engine powered cars have recently become subject to considerable negative publicity for toxic emissions they produce. Heating air in an engine produces nitrogen oxides (NO_x) which include the toxic nitrogen dioxide (NO_2), greenhouse gas nitrous oxide (N_2O) and nitric oxide (NO), which reacts with oxygen to form NO_2. Long-term exposure to nitric oxide can significantly increase the risk of respiratory problems. The fine particulate matter (PM) that IC engines produce also causes cancer and can have acute respiratory effects. So, technologies have been developed to control and reduce these pollutants. A significant development has been made especially in last 20 years. While new ways for a sustainable emissions-free mobility are being discussed, discovered and developed, it is expected that the internal combustion engine will remain the dominant power source for many years to come, and with the right balance of technologies and innovations we can make ICE-based powertrains cleaner than ever before. This study presents these concepts along with the recommended technologies to meet the upcoming emission targets i.e EU7 standards. Further investigation is on-going into optimising these systems and also exploring novel ideas and innovative technologies to go beyond EU7 and achieve near-zero emissions.

36. An Interference-Free Laser-Based Methane Sensor Using Cepstral Analysis

Mhanna Mhanna, Mohamed Sy, Aamir Farooq

King Abdullah University of Science and Technology, Saudi Arabia

A mid-infrared laser-based sensor is designed and demonstrated for quantification of methane concentrations. The sensor is based on a distributed feedback inter-band cascade laser (DFB - ICL) operating near 3.3 μm. Wavelength tuning with cepstral analysis was employed to isolate methane absorbance from (1) fluctuations/errors in the baseline laser intensity (I0), and (2) interfering absorbance of benzene. Cepstral analysis creates a modified form of the time-domain molecular free-induction-decay (m-FID) signal to temporally separate optical and molecular responses. Methane concentration is determined by least-squares fitting a simulated absorbance m-FID signal of the target species to the measured absorbance in the time domain. The developed sensor is insensitive to baseline laser intensity imperfections and benzene interference, which vary slowly in the frequency domain and thus decay rapidly in the time domain. Accurate measurements of methane in the presence of benzene were performed by careful selection of scan index (ratio of laser tuning range to spectral linewidth) and initial and final time of fitting the m-FID signal. The sensor can be utilized to measure methane concentrations in harsh environments and in the presence of interfering species.

37. Experimental Study on the Swirling Flame Combustion of Heavy Fuel Oil/Water Emulsion

Felipe Campuzano, Kai Xu, Earnesto Thachil, Ettouhami Es-sebbar, Saumitra Saxena, William Roberts

King Abdullah University of Science and Technology, Saudi Arabia

Ibrahim Al Ghamdi, Mohammed Al Qahtani

Saudi Electric Company, Saudi Arabia

Due to its high energy density, low cost, and extensive availability, heavy fuel oil (HFO) is considered an interesting alternative fuel for use in combustion systems, either for power generation or transportation (i.e. in the marine sector). However, HFO is very difficult to burn, leading to the formation of pollutants (e.g. particulate matter, soot, cenosphere, etc.) that may cause detrimental effects not only to the combustion systems themselves, but also on the environment. In order to improve the combustion process of HFO and therefore reduce the formation of hazardous pollutants, an attractive pathway to enhance its performance is to emulsify HFO with water. In this regard, the present investigation addresses fundamental, as well as practical aspects of the combustion of HFO-water emulsions under swirling-flame conditions, which aim to mimic the combustion process in typical industrial-scale boilers. Emulsions were prepared via sonication, and samples with water contents of 0 (pure HFO), 5, 10, 15, 20, and 30 wt. % were obtained. The combustion experiments were carried out in a lab-scale burner with an air-blast nozzle and swirling airflow, which generates an environment similar to the one in real boiler burner operation. Laser diagnostics were implemented in order to gain insights regarding the impact of micro explosion phenomena on soot, cenosphere, and particulate matter (PM) formation during the combustion of emulsified HFO. Furthermore, advanced analytical techniques, including Scanning Electron Microscope (SEM) and X-Ray Photoelectron Spectroscopy (XPS) were utilized to study the fundamental characteristics (morphology, structure, sulfur content, etc.) of the PM/cenosphere collected from the experimental campaign. Experiments showed that the emulsified HFO flame tends to be very unstable for water contents higher than 15 wt.%, and even hard to maintain when this content is 30 wt.%. The addition of 15 wt. % of water in HFO resulted in a decrease in the soot concentration and size, which was attributed to the micro-explosion phenomenon taking place during the emulsified HFO combustion. Similarly, micro-explosions seem to induce the conversion of thiophene constituents (dominant sulfur-containing compounds in the collected PM) into sulfones due to better oxidation characteristics. Overall, the obtained results presented in this study aim to provide fundamental knowledge needed to implement HFO-water emulsions on an industrial scale.

38. Stability limits and emission performance of ammonia-methane swirl flames for future power generation

Marwan Abdullah, Mourad Younes, Aqil Jamal

Saudi Aramco, Saudi Arabia [2]

Cristian D. Jimenez, , Thibault Guiberti, Bandar Solami, William Roberts,

King Abdullah University of Science and Technology, Saudi Arabia

Synthetic fuels such as ammonia (NH3) hold good promises to support the power generation sector decarbonization due to their ease of transport and carbon-free nature. Considering the challenges associated with pure ammonia combustion and the gradual uptake or adoption of ammonia in the utility sector, it would be interesting to investigate ammonia/methane cofiring. Several NH3 volume fractions in the fuel blend, ranging from 0 to 1, were tested to investigate the swirl flames' stability limits and exhaust NO emissions at elevated pressures in a reduced-scale burner that mimics features of a current commercial gas turbine burner. The study covered a wide range of equivalence ratios to identify promising operating conditions. The experiments demonstrated a significant abatement potential of CO2 emissions when adding ammonia to the fuel blend. NO and N2O emissions levels decreased for rich equivalence ratios. Future work assessing unburnt NH3 in rich operation and optimizing burner design after-treatment consideration would help advancing ammonia adoption in the utility sector.

39. Stability Limits and Emissions of Double Swirl Burner with Methane/Ammonia blends

Alfaisal Albalawi, Ayman Elbaz, William Roberts

King Abdullah University of Science and Technology, Saudi Arabia

Khalid Mojallid

King Abdulaziz University, Saudi Arabia [2]

The transition to zero net carbon emissions is of the utmost importance to combat the future of global warming. Ammonia has gained wide attention as being a carbon-free energy source and potential to be a hydrogen carrier due to its ease of transportation and low manufacturing cost. However, ammonia has drawbacks that must be addressed before its broad implementation as a fuel, such as a narrow flammability limit, slow reactivity, and corrosiveness to certain materials. This study investigates the flame stability limits and emissions of swirling flame issued from a newly designed double staged swirl burner. This burner has two concentric swirlers to allow for the burning of two reactant streams (inner and outer) with different equivalence ratios, velocity ratios and powers. In the first part of the study, a parametric study is conducted by varying the two streams equivalence ratio, power and bulk velocity. The stability limit of the flame was assessed by determining the flashback limit and lift-off of the flame. Next, emission measurements were conducted at the exhaust to determine NOx, CO, and unburned hydrocarbons levels under different flow conditions.

40. Experimental Investigation of Soot Formation at Elevated Pressure in Laminar Inverse Diffusion Flames

Peng Liu, Ibrahim Alsheikh, Sreenivasa Rao Gubba, Saumitra Saxena, William Roberts

King Abdullah University of Science and Technology, Saudi Arabia

Obulesu Chatakonda,

Air Products Technology Center, Saudi Arabia

Jeffrey W Kloosterman,

Air Products and Chemicals, Inc., USA

Experimental investigation of laminar inverse diffusion flames have been carried out at elevated pressures to understand the effect of O2 concentration on soot formation. The fuel stream consists of a mixture of methane and CO2, and the oxidant stream consists of O2 and N2. Diagnostic methods such as Laser-Induced Incandescence (LII) and Luminescence were employed. These techniques were used to probe soot volume fraction (SVF) and OH* intensity signals. Four sets of experiments were carried out at 4 bar to observe the effects of varied O2 concentrations. In experiments, the O2 concentrations were varied (70%, 58%, 46%, and 33% by volume) while the total oxidant stream was kept constant (i.e. 800 mL/min). Flowrates for both CH4 and CO2 were kept constant (1200 mL/min and 800 mL/min, respectively). Results reveal that soot loading in inverse co-flow flames decreases as O2 concentration increases.

41. Soot formation in ammonia-hydrocarbon combustion

Peng Liu, William Roberts

King Abdullah University of Science and Technology, Saudi Arabia [1]

An intermediate step in the transition to hydrogen and ammonia is the blending of these fuels with hydrocarbons. In this talk, soot formation in laminar counter-flow flame, laminar co-flow flame, and turbulent jet flame fueled with ammonia-hydrocarbon are presented. Soot reduction is observed from flame experiments. To understand the physics, pyrolysis experiment is conducted for HCN-C2H2-N2 mixture. The results highlight the important of HCN on soot reduction. Our quantum chemistry calculation further reveals that the reaction activity of HCN is as completive as C2H2 on polycyclic aromatic hydrocarbon growth, which is regarded as soot precursor.

42. Elucidating First Stage Ignition Chemistry of Dimethyl Ether using a Laminar Flow Reactor

Awad Alquaity,

King Fahad University of Petroleum and Minerals, Saudi Arabia

Antonio Attili,

University of Edinburg, United Kingdom

Heinz Pitsch,

Aachen University, Germany

Advanced low-temperature combustion engines with the potential to reduce emissions are controlled predominantly via chemical kinetics which necessitates the use of kinetic models that are well-validated over a wide range of conditions. This talk focuses on the characterization of a custom-built laminar flow reactor (LFR) capable of investigating the ignition chemistry of fuels in the low-temperature regime (<720 K). The flow reactor is used to measure the first-stage ignition delay locations and species mole fractions for stoichiometric dimethyl ether/O2/N2 mixtures at temperatures between 541 to 592 K. To complement the experimental measurements, simulations were carried out using the in-house FlameMaster code to understand the combustion behavior in the flow reactor and to predict the ignition locations and species mole fractions for different experimental conditions. The ability of the LFR to measure derived ignition delay times of up to 3.3 seconds extends the range of conventional homogeneous reactors such as shock tubes and rapid compression machines significantly and provides complementary data to further constrain kinetic models.

43. A step toward quantitative planar laser-induced fluorescence of hydroxyl radical in hydrogen-fueled detonations

Karl Chatelain, Samir B. Rojas Chavez, Thibault F. Guiberti, **Deanna A. Lacoste**

King Abdullah University of Science and Technology, Saudi Arabia

Rémy Mével

Tsinghua University, Beijing, China

Recently, hydrogen-fueled detonations have a growing interest due to their thermodynamically more efficient combustion cycles, the use of carbon-free fuels, and the potential role of hydrogen in the circular carbon economy. Compared to classical flame diagnostics (i.e., deflagration regime), a limited number of laser diagnostics were employed to perform two-dimensional (2D) quantitative measurements in detonations. This lack of quantitative information currently prevents the validation of multidimensional numerical simulations and the development of the next-generation, low-carbon and highly efficient, power generator (i.e., detonation engines).

In this study, we investigated the effect of the excitation line on the planar laser-induced fluorescence of hydroxyl radical (OH-PLIF) imaging in H2-detonations. From these results, we validated our in-house spectroscopic code, called KAT-LIF, with experimental results obtained in our optical detonation duct (ODT). We numerically investigated the effect of the initial conditions, N2- or Ar-dilution, and excitation lines on the OH-LIF measurements (emission spectrum, fluorescence intensity, and OH concentration). Also, we experimentally evidenced better excitation strategies to obtain qualitative information far from the front. Besides these new excitation strategies are mainly valuable for qualitative validations of numerical simulations, they may also open a path toward OH-PLIF quantitative measurements in detonation waves.

44. Dual-camera high-speed imaging of ethanol combustion in a high-pressure shock tube

Miguel Figueroa Labastida, Touqeer Anwar Kashif, Aamir Farooq

King Abdullah University of Science and Technology, Saudi Arabia

Preignition, which leads to non-homogeneous combustion in otherwise ideal reactor conditions has been observed in shock tubes, drifting the performance of these facilities away from ideal operation and, therefore, jeopardizing the accuracy of the measurements being taken. We present simultaneous lateral and endwall high-speed imaging experiments of the combustion of ethanol at high pressures. A novel optical section for the High Pressure Shock Tube (HPST) at KAUST was designed, manufactured and tested. This section allows the visualization of combustion phenomena through the endwall and sidewall, providing axial and radial homogeneity information. Experiments at high temperatures showed homogeneous fast ignition, while inhomogeneities could be observed at lower temperatures. The use of helium as bath gas was tested as a potential non-ideality mitigation measure. Results using He did not show significant difference to those using Ar. To our knowledge, this is the first report of dual-camera high-speed imaging of combustion in high pressure shock tubes.

45. A laser diagnostic for HCN detection in mid-infrared

Ali Elkhazraji, Mohammed Adil, Mohammad Khaled Shakfa, Binod Raj Giri, Aamir Farooq

King Abdullah University of Science and Technology, Saudi Arabia

In light of the challenges faced by our world due to global warming, zero-carbon fuels are becoming very important to reduce carbon dioxide emissions. One promising candidate of such fuels is ammonia which has been investigated in recent years for its use in power generation and transportation. In order to better evaluate the performance of ammonia as a fuel, it is important to develop chemical kinetics models which are capable of accurately depicting ammonia combustion. This calls for new diagnostics suitable of measuring different intermediates involved in ammonia combustion to measure relevant reaction rate constants and/or to improve the fidelity of predictive chemistry models.

The significantly low reactivity of ammonia makes it incompatible for direct use in many combustion systems. One of the strategies to overcome that is to blend it with a combustion promoter such as hydrocarbons. An important intermediate of ammonia/hydrocarbon combustion is hydrogen cyanide (HCN). In particular, being the main source of nitrogen for NOx formation, HCN is the main NOx precursor from the fuel-bound nitrogen. It is believed that HCN is the reason why ammonia/hydrocarbon flames produce more NOx compared to pure-ammonia flames. The current techniques for measuring HCN in reactive experiments are based on gas chromatography and UV lasers. Here, we report a mid-IR laser-based HCN diagnostic for shock tube chemical kinetic studies. The custom-designed laser is based on difference-frequency generation (DFG) and makes use of a nonlinear orientation-patterned GaAs crystal to generate an idler beam (tunable in the range 11.58 - 15 μm) as a result of the DFG process between a CO2 gas laser and an external-cavity quantum cascade laser. The targeted HCN absorption peak is its most intense IR peak, namely, ν_2, at 712 cm-1. This wavelength choice allows for a more selective sensing of HCN compared to the ν_3 band near 3300 cm-1 where many hydrocarbons have their C-H stretching modes, and a more sensitive sensing than the ν_1 band near 2090 cm-1 whose relative intensity is significantly less than that of the ν_2 band.

We report HCN pressure-dependent absorption cross-section measurements over 712 - 715 cm-1 and pressure range of 50 - 1000 Torr. We also performed temperature-dependent absorption cross-section measurements where HCN/argon mixtures were shock-heated to 900 - 3000 K at 714.5 cm-1 which is predicted to be the strongest IR peak of HCN at high temperatures. We then used these results to measure HCN formation in a reactive experiment of isoxazole decomposition behind reflected shocks. The measured time-histories of the formed HCN are compared with kinetics simulations to evaluate rate coefficient of isoxazole decomposition.

46. Characterization of a Cassegrain optical system for spatially-resolved measurements of flame chemiluminescence spectra

Amjad Aljarallah, Oneil Goisot, William Roberts, Thibault Guiberti

King Abdullah University of Science and Technology, Saudi Arabia

This study reports on the characterization of an optical system based on a Cassegrain lens and designed to enable spatially-resolved measurements of flame chemiluminescence. Chemiluminescence occurred from excited radicals naturally present in laminar methane-hydrogen-air diffusion flames stabilized with a counterflow burner. The Cassegrain lens was connected to a spectrometer via a UV-capable optical fiber. First, the spatial resolution of the optical system was assessed for different diameters of the optical fiber core, 100, 200, and 400 μm. It was found that the spatial resolution of the optical system is equal to the diameter of the optical fiber core as long as the latter is larger than or equal to 200 μm, below which spatial resolution is limited by the Cassegrain lens itself and is 200 μm. Second, spatially-resolved chemiluminescence spectra were recorded along the burner axis, i.e., along the normal of the flame front, for different fuel blend compositions. In this study, the volume fraction of methane in the methane-hydrogen fuel blend was varied from 10 to 90% by increments of 20%. Experiments were conducted for a fixed strain rate of 150 /s. Consistent with existing literature, contributions from OH*, CH*, and C2 excited radicals were observed in all cases. However, relative intensities of chemiluminescence from these three excited radicals and the spatial location where they peak were found to vary significantly with the fuel blend composition. Of particular interest is the fact that OH*, CH*, and C2 intensities do not always peak at the same location. For example, increasing the hydrogen fraction in the fuel blend increases the separation distance between OH* and CH* peaks. Third, measurements were compared with simulations achieved with the opposed flame module of Chemkin and a previously validated detailed kinetic mechanism accounting for OH* and CH* excited radicals. It was found that simulations and measurements exhibit the same trends of chemiluminescence intensity and OH*/CH* peak separation distance when the fuel blend composition is varied, as long as the spatial resolution of the optical system is accounted for in the simulations by spatial convolution with the instrument function. Based on this agreement, it was concluded that the optical system performed as intended and to high standards. Therefore, preliminary experiments were conducted for an ammonia-hydrogen-air diffusion flame for which no validated detailed kinetic mechanism accounting for excited radicals exist. These data will be used in the future to validate a new kinetic mechanism for ammonia flames.

47. Laser-induced Fluorescence of NO in Laminar and Turbulent Ammonia-Hydrogen-Nitrogen Diffusion Flames at High Pressure

Guoping Wang, Hao Tang; Chaobo Yang; Gaetano Magnotti; Thibault F. Guiberti; William L. Roberts

King Abdullah University of Science and Technology, Saudi Arabia

Ammonia combustion is a very promising carbon-free combustion strategy, but NOx emission in ammonia applications is one of the most challenging problems. This work developed a one-dimensional laser-induced fluorescence (LIF) method to measure the NO mole fraction in ammonia-hydrogen diffusion flames quantitatively. We choose the A^2 Σ^+-X^2 Π (0-1) excitation at 236 nm to avoid the absorption of the 226-nm ultraviolet laser by ammonia. In the experiment, NO-LIF and Raman scattering are measured simultaneously. Based on the measured LIF signal, flame temperature, and major species, we developed a LIF calibration method suitable for diffusion flames. Nitrogen dilution is used to study the effects of temperature on the NO mole fraction in ammonia-hydrogen flames. The results show that although the flame peak temperature ranges from 1835 K to 2342 K across all tested conditions, the peak NO mole fraction only slightly changes. This indicates that the main NOx formation mechanism is fuel NOx rather than thermal NOx. Controlling the temperature of the reaction zone is not an efficient strategy to reduce NOx emissions from flames with ammonia in the fuel blend. Furthermore, we studied the NO emission of ammonia-hydrogen-nitrogen jet diffusion flames with 14% and 28% cracking ammonia. All the flames are measured at micro gas turbine relevant-pressure of 5 bar. The results provide the mean and RMS distributions of NO from 1D to 40D. The NO concentration can reach 104 ppm at 1D and slightly decreases to about 103 ppm at 40D. The quantitative data set of NO, major species and temperature can be used for validating the NOx production in numerical simulations.

48. On the accuracy of CO/H2 Kinetic Mechanisms for Prediction of Syngas Non-premixed Flames Characteristics

Sayed Mughees Ali,

Eindhoven University of Technology, Netherlands

Gasification is a widely used thermo-chemical route for conversion of biomass and coal, yields fuel gases rich in carbon monoxide and hydrogen (called syngas or producer gas). Due to the toxic nature of CO, an accurate kinetic mechanism is required for the prediction and control of its emission from gasification-based combustion devices (domestic and commercial scale biomass-based cooking devices, stationary gas turbines, industrial furnaces etc.). CFD simulation results from earlier studies clearly depict the incapability of available kinetic mechanisms for the prediction of the Sandia-ETH Zurich turbulent syngas jet diffusion flames characteristics. The two main reasons for this inaccuracy are, (1) modelling of turbulence-chemistry interactions, (2) optimization of kinetic mechanism rate parameters. To check the accuracy of kinetic rate parameters of available CO/H2 kinetic mechanisms (5 detailed and 3 short kinetic mechanisms) for syngas non-premixed flames, a simplfied canonical configurations namely; laminar jet diffusion is studied both experimentally and computationally. The flame height comparison of 6 different compositions of CO/H2 laminar jet diffusion flames showed that none of the mechanisms is capable of accurately predicting experimental flame height and thus highlight a need for a new optimized kinetic mechanism for Syngas combustion.

49. Surrogate Formulation and Chemical Kinetic Modeling of Vacuum Residual Oil

Mohammed AlAbbad, Ribhu Gautam, Xiaoyuan Zhang, Muralikrishna Khandavilli, Saumitra Saxena, Mani Sarathy

King Abdullah University of Science and Technology, Saudi Arabia

Obulesu Chatakonda,

Air Products Technology Center, Saudi Arabia

Joshua Middaugh

Air Products and Chemicals, Inc, USA

Residual fuel oils are receiving increasing attention from the power generation sector and chemical industry. Gasification is an approach for converting large complex hydrocarbons to syngas, a mixture of carbon monoxide (CO) and hydrogen (H2), and then syngas can be purified and converted to H2 as a clean zero-emission fuel.

Detailed chemical kinetic mechanisms are needed to simulate the gasification process for the purposes of design and development. Simulations such as computational fluid dynamics (CFD) provide a promising approach for the development of complicated processes such as internal combustion and heavy oil gasification. Petroleum-based fuels contain hundreds to thousands of components. The complexity of these fuels increases as moving from lighter (natural gas) to heavier (residual fuel oils such as vacuum residual oil (VRO)) hydrocarbons. The compositions of these fuels vary according to the refining process and the geographic sources. Including all the components of a fuel in a detailed chemical kinetic model is very challenging. Also, fundamental data such as rate constants, reaction paths and thermodynamic parameters are still not available for many of these components. Therefore, to solve such a challenge, a simple surrogate with a minimum number of components can be proposed. The surrogate can be formulated by matching the functional groups and some critical characteristics of the fuels, such as average molecular weight and H/C ratio.

In this work, a three-component surrogate is proposed for VRO. The target of the surrogate is to replicate the important chemical properties of VRO and also match some physical properties. The Nuclear magnetic resonance (NMR) data was used to match the functional groups of the fuels. Elemental analysis and Fourier-transform ion-cyclotron-resonance mass spectrometry (FT-ICR MS) data was used to match the average molecular weight (AMW) and average molecular formula. For detailed chemical kinetic development of such a complicated fuel, a combination of functional groups for mechanism development (FGMech) [1,2] and hybrid chemistry (HyChem) [1] methodology was used. The kinetics of the thermal pyrolysis of the fuel is modeled using lumped kinetic parameters extracted from experiments and FGMech approach, whereas the oxidation of the pyrolysis products

is described by their detailed chemical models. The model is validated and in good agreement with industrial data of Orimulsion gasification pilot plant.

References:

[1] Wang, H., Xu, R., Wang, K., Bowman, C. T., Hanson, R. K., Davidson, D. F., ... & Egolfopoulos, F. N. (2018). A physics-based approach to modeling real-fuel combustion chemistry-I. Evidence from experiments, and thermodynamic, chemical kinetic and statistical considerations. Combustion and Flame, 193, 502-519.

[2] Zhang, X., Yalamanchi, K. K., & Sarathy, S. M. (2021). A functional-group-based approach to modeling real-fuel combustion chemistry-I: Prediction of stoichiometric parameters for lumped pyrolysis reactions. Combustion and Flame, 227, 497-509.

[3] Zhang, X., & Sarathy, S. M. (2021). A functional-group-based approach to modeling real-fuel combustion chemistry-II: Kinetic model construction and validation. Combustion and Flame, 227, 510-525.

50. Global chemical kinetics of HFOs pyrolysis for practical applications

Elia Colleoni, Paolo Guida, Saumitra Saxena, William Roberts

King Abdullah University of Science and Technology, Saudi Arabia

Tiziano Faravelli, Alessio Frassoldati

Politecnico di Milano, Italy

While the energy demand is continuously growing, the high-quality oil feedstock is constantly depleting across the globe. Heavy Fuel Oils (HFOs) are expected to play a vital role in filling the gap of future energy demand and supply chain. However, further research is required to upgrade and burn HFOs in order to mitigate current emissions legislations. HFOs are generally separated into four main fractions Saturates, Aromatics, Resins, and Asphaltenes (SARA). This work presents a predictive approach to model HFO pyrolysis. The idea is to develop models for the pyrolysis of each SARA fraction, and finally, reproduce the pyrolytic behavior of a generic HFO as the weighted sum of its SARA fractions contribution. The first step in the development of the pyrolysis model is in defining the characterization framework. HFOs, as well as their fractions, are complex mixtures made by thousands of compounds. Therefore, it is indispensable to find an effective way to create a surrogate blend that can be used to perform simulations. Surrogate blends are defined for each SARA and the formulation is based on the elemental composition of each fraction.

The development started with extensive literature research to find as much information as possible on the elemental compositions of each SARA extracted from different oil feedstocks. A database with 208 data for Asphaltenes and more than 100 for Resins was built. Much fewer data were found for Saturates and Aromatics. Based on the samples collected in the literature pseudo components of each fraction were designed to be as realistic as possible. The second step of the work was the definition of a pyrolysis pathway for each pseudo-components. Pyrolysis is a phenomenon that involves a large number of different reactions and species, following complicated pathways. To reduce the complexity of the model the pyrolysis behavior of each pseudo-component is modeled with an irreversible first-order reaction with the task of approximating the overall kinetics. The reaction network leads to the formation of gas and solid (CHAR) products. Products were defined according to chemistry-related considerations. Stoichiometric coefficients, activation energy, and pre-exponential factor for each pseudo-component reaction are derived from a fitting data approach of TGA experiments and gas distributions obtained from pyrolysis experiments. The model obtained is predictive and versatile in reproducing the pyrolytic behavior of different oil samples.

51. Kinetic and product analysis of the pyrolysis of Salicornia bigelovii under CO2 and N2 atmospheres

Jinan Aljaziri, Ribhu Gautam, Sultan Alturkistani, Mani Sarathy

King Abdullah University of Science and Technology, Saudi Arabia

The challenges associated with biomass availability in arid regions can be eliminated by using halophytes such as Salicornia bigelovii (SB). SB biomass has the ability to grow in arid climates using brackish or seawater for irrigation. Biomass pyrolysis results in many gases such as CO2, CH4, H2, and CO. Recycling CO2 back to the process can increase the economic viability of that process. Furthermore, pyrolysis under CO2 atmospheres can aid in mitigating CO2 emissions released to the environment. This study focuses on understanding the effect of CO2 atmosphere on the pyrolysis of SB by performing a detailed kinetic analysis as well as investigating the pyrolysis products. Pyrolysis of SB was performed in a quartz tube reactor at a temperature of 550 °C under both CO2 and N2 atmospheres. Pyrolysis in CO2 resulted in a 10% increase in the bio-oil yield (~60 wt.%), whereas char yields were unaffected (~21 wt.%). The bio-oil and biochar were collected and characterized. Gas chromatography/mass spectrometry analysis of the bio-oil showed that CO2 pyrolysis enhanced the amounts of acids along with amines/amides compared to bio-oil from N2 pyrolysis. The elemental composition of the biochar showed a 6.5% increase in carbon and a 5.8% decrease in oxygen due to the presence of CO2 in the pyrolysis atmosphere. In addition, an FT-IR analysis of the biochar indicated that CO2 inhibited the volatilization of certain functional groups, such as phenols, tertiary alcohols and aromatics. Furthermore, biochar generated in CO2 environment exhibited a specific surface area 12 times larger than that produced from N2 pyrolysis. Mass loss profiles were acquired for SB in a Thermogravimetric analyzer (TGA) under both atmospheres. Non-isothermal kinetic analysis was initially performed by splitting the decomposition of SB into three different reaction regions under both CO2 and N2 atmospheres. The analysis revealed that CO2 lead to an increase in the average apparent activation energy from 146.5 kJ mol-1 in N2 to 163.4 kJ mol-1 in CO2. The kinetic model function of the process has been determined and parameterized as well as the pre-exponential factor.

52. Investigating 1, 3-butadiene kinetics using UV absorption spectroscopy

Dapeng Liu, Aamir Farooq

King Abdullah University of Science and Technology, Saudi Arabia

1,3-Butadiene is not only a crucial intermediate in large hydrocarbon pyrolysis and oxidation, but it also makes a difference to the formation and growth pathway of poly-aromatic hydrocarbons (PAHs). The quality of kinetic studies is degraded by the inabilities of previous diagnostic techniques, such as resolution (high concentration) and diagnostic condition (low temperature). In this work, we achieve quantitative 1,3-butadiene measurement using laser absorption spectrometry at 212.5 nm. The 1,3-butadiene absorption cross-sections are appropriately measured with three gas mixtures behind the reflected shock wave for temperatures below 1820 K and pressures around 1 bar. The cross-section values from three different gas mixtures agree well and are fitted in the expression below ($cm^2molecule^{-1}$):

σ(1,3-BTD, 212.5nm)=2.397×10^{-23} T^2-$8.407\times10^{-20}\times T+9.483\times10^{-17}$, R^2=0.995

The current diagnostic scheme not only shed light to high-temperature 1,3-butadiene kinetic experiments, but could also provide valuable validation targets to relevant models such as Aramco 3.0. A preliminary representative experiment is conducted to study the 1,3-butadiene decomposition, and the overall decomposition rate coefficients are given (s^{-1}):

$k=1.68\times10^{9}\ e^{-21188.5/T}$

The determined rate coefficients are compared with extensive literature measurements as well as kinetic models. The rate coefficients from the current work show reasonably good agreement with literature calculations with slightly smaller activation energy.

Saudi Arabian Section of the Combustion Institute