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ASPACC 2023 Paper Abstracts

Towards Net-Zero Carbon & Data-Driven Future

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Paper ID: 12

Numerical study of ammonia-hydrogen premixed ball-like flame

Wai Siong Chai (National Sun Yat-Sen University), Lei Zhou (Harbin Institute of Technology)

This work evaluates the combustion characteristics of premixed ammonia-hydrogen (NH_3/H_2) mixtures numerically in a three-dimensional model under gravity conditions with the aid of Okafor mechanism. Effects of hydrogen ratio, equivalence ratio and total flow rate on combustion and emission characteristics were investigated. Numerical results are validated and are in general agreement with experimental data. NH_3/H_2 mixture tends to burn to form a ball-like flame at low flow rate, low equivalence ratio and high hydrogen ratio. Results showed that the temperature of the NH_3/H_2 premixed flame is the lowest under flame ball formation conditions. The temperature of the NH_3/H_2 premixed flame increases with the flow rate and equivalence ratio, peaking at φ=1.0, while decreases with hydrogen percentage. Analysis of the effect of equivalence ratio on NO_x showed that minimum NO_x emissions and unburned ammonia are at slight rich condition. NO_x decreases and then increases with flow rate.

Paper ID: 13

Numerical investigation and adjustment on the ignition delay mechanisms of ammonia-based fuels

Wai Siong Chai (National Sun Yat-Sen University), Lei Zhou (Harbin Institute of Technology)

In this study, three typical ammonia-based fuels, ammonia, ammonia-hydrogen and ammonia-methane, are numerically simulated for ignition delay time, and the applicability of different ammonia-based fuels mechanisms is examined and analyzed. The important reactions in the mechanisms are analyzed by sensitivity. The best mechanism selection for each case was obtained. Based on the Glarborg mechanism, the reaction coefficients of some radicals containing CH_3 radicals were updated for ammonia-methane ignition. The adjusted mechanism can simulate the ignition delay time of three ammonia-based fuels well and improve the prediction of NH_3/CH_4 ignition delay time with an average error of 3.54% from the experimental value.

Paper ID: 17

Partial oxidation of H_2S: a kinetic modeling study and characterization of important reactions with quantum chemistry calculations

Manuel Monge Palacios (King Abdullah University of Science and Technology), Qi Wang (King Abdullah University of Science and Technology), Amjad Shaarawi (Exploration and Petroleum Engineering Center-Advanced Research Center), Adrian Cavazos Sepulveda (Exploration and Petroleum Engineering Center-Advanced Research Center), S. Mani Sarathy (KAUST)

We developed a new kinetic model for the pyrolysis and oxidation of H_2S by merging former models. The new model covers a wider range of conditions than the original ones, including pyrolysis and oxidation in the presence of CO_2. Our purpose is the determination of the most prominent reactions of the species H_2S, H_2, and SO, as well as the conditions that maximize the H_2 yield. Those reactions were identified by means of a rate of production and sensitivity analysis, concluding that the SO species is a key intermediate in H_2S partial oxidation under rich conditions. Additionally, we performed quantum chemistry calculations to characterize the potential energy surface and describe the reaction mechanism of three of those important reactions whose rate constants had been set in former models by means of analogies. This work is the first step of a kinetic

study that is aimed at improving the newly merged kinetic model.

Paper ID: 19

Effects of gas-phase diffusion transport on solid-state combustion synthesis

Chun-Liang Yeh (Feng Chia University), Kuan-Ting Liu (Feng Chia University)

TiB_2–TiC–Al_2O_3 and ZrB_2–ZrC–Al_2O_3 ceramic composites were produced via PTFE-activated combustion synthesis involving low-exotherm thermites. PTFE (Teflon) played a dual role in promoting the reaction and carburizing reduced Ti and Zr. The threshold amount of PTFE for the TiO_2/Al-based reaction was 2 wt% and for the ZrO_2/Al-based reaction was 3 wt%. The addition of PTFE led to the formation of gas-phase transport species, which activated the solid-state combustion reaction. The increase in PTFE increased the combustion velocity and temperature. The TiO_2/Al-based reaction was more exothermic than the ZrO_2/Al-based reaction and exhibited a faster combustion rate and lower activation energy. Both triplex composites displayed mixed microstructures consisting of short-rod borides, spherical carbides, and Al_2O_3 agglomerates.

Paper ID: 20

Selective BTEX detection using laser absorption spectroscopy in the CH bending mode region

Ali Elkhazraji (KAUST), Joury Aldhawyan (KAUST), Mhanna Mhanna (KAUST), Mohamed Sy (KAUST), Mohammad Adil (KAUST), Mohammad Khaled Shakfa (KAUST), Aamir Farooq (KAUST)

We report the development of a selective BTEX (benzene, toluene, ethylbenzene, and xylenes) laser-based sensor in the long-wavelength mid-infrared spectral region. The sensor probes the CH bending modes of BTEX taking advantage of the strong, spectrally isolated absorption features of aromatics in this spectral region. Measured mole fractions are validated against manometric measurements.

Paper ID: 21

General correlation of laminar burning velocities for multicomponent syngas (H_2/CO/CH_4)/air mixtures

Tien Minh Nguyen (The University of Danang), Le Chau Thanh Nguyen (The University of Danang), Tan Thong Ngo (The University of Danang), Phu Nguu Do (The University of Danang), Duy Quoc Tong (The University of Danang), Phuoc Dinh Tran (The University of Danang)

A thorough understanding of the combustion characteristics of multicomponent synthesis gas (syngas) plays an important role in the further development of syngas-fueled applications. This study investigated the laminar burning velocity (S_L) of multicomponent syngas/air and its general correlation using the pressure rise method. Lean multicomponent syngas/air mixtures at various equivalence ratios (f = 0.6, 0.7, 0.8) containing different volumetric fractions of H_2 (10–30%), CO (10–30%), and CH_4 (40–60%) were conducted in a cylindrical constant volume combustion chamber using a dual-coil car ignition system. The result indicated that S_L value was maximum at a (H_2/(H_2+CO)) ratio of 0.5, at which the CH_4 content was the lowest. Beyond this ratio, the value of S_L decreases, suggesting a significant influence of CH_4 concentration. The current S_L values, together with previous syngas data, could be well represented by a modified correlation with a slight discrepancy. This suggests a possible self-similar propagation of syngas/air laminar flames, regardless of the equivalence ratio, constituent fraction, temperature, pressure, and dilution.

Paper ID: 22

A pilot research of re-defining what is 'flashover'

Han Shun Hsu (National Fire Agency), Ricky Carvel (University of Edinburg), Chia Lung Wu (Chang Jung Christian University)

'flashover' is an dominant term in fire safety society, which been described as a critical point to differentiate compartment fire into 'pre flashover' and 'post flashover'.Moreover, in the fire design process, fire safety engineering related guidance simply addressed once the Heat Release Rate (HRR) reaches the value to have flashover, and the HRR of that compartment will rise into the peak instantly then reach the fully developed phase. However, there are a variety of criteria and descriptions of flashover even though the society recognized it as a crucial pare meter, therefore, this research aims to collect existing criteria and descriptions toward flashover, then to provide an overview of possible re-definition of flashover in conclusion.

Paper ID: 23

Modified multiflame model for AP-HTPB composite propellant combustion

Neeraj Kumar Pradhan (Indian Institute of Technology Bombay), Arindrajit Chowdhury (Indian Institute of Technology Bombay), Debasis Chakraborty (Mahindra University, Hyderabad), Neeraj R Kumbhakarna (Indian Institute of Technology Bombay)

Among composite solid propellants, AP/HTPB is the most widely used. Modeling of the burn rate of this heterogeneous propellant composition is an active research area with new models continuously being formulated. Amongst the many models proposed in the literature, BDP or Cohen and Strand formulations are mostly used to predict the burn rate. A modified model is proposed in the present work. The modifications include (1) Three flame structure with different surface temperatures for oxidizer and binder, (2) Detailed energy balance equations at surfaces, (3) Modified surface heat release term, (4) Flame temperature as a function of initial temperature, pressure, and fuel/oxidizer ratio, (5) Modification of diffusion stand-off distance. The predicted burn rates are compared with experimental and other theoretical results of AP monopropellants, AP-HTPB monomodal, and multimodal configurations. Better predictions than the the existing ones are observed in all the cases.

Paper ID: 24

Experimental study on non-reactive flow characteristics of a novel multi-swirl lean direct injection burner

Sarath Perikathra (Indian Institute of Technology Madras), Muruguanandam T M (Indian Institute of Technology Madras.)

A novel multi-swirl lean direct injection (LDI) burner, incorporating several lean direct injection modules, has been developed for low-emission aero-propulsion systems. This paper investigates the detailed analysis of the non-reacting flow characteristics of this burner and makes an effort to explain the salient features of this system. Stereo PIV was used to measure the non-reacting flow fields in the axial plane of the burner at different axial distances from the burner plate. Examination of averaged flow fields obtained from the sPIV shows the strong interaction of the swirling flows emerging from the neighboring swirlers, which may help efficient fuel mixing. The computed mean axial and swirl velocity plots imply high swirl flow and strong interactions. High

turbulent flow structures are formed at the interface of the adjacent swirlers because of opposing flow directions, and interactions of these structures might play an effective role in flame stabilization.

Paper ID: 25

Combustion analysis of a micro gas turbine combustor with CH_4/NH_3 fuel blends

Sz-Pei Ho (Chang Gung University), Cheng Cheng (Chang Gung University), Hsin-Yi Shih (Chang Gung University)

Ammonia has been proposed as a potential alternative fuel to achieve low-carbon emissions. However, compared to typical hydrocarbon fuels, due to their combustion characteristics of low reactivity and higher NO_x emissions, maintaining stable ammonia combustion in industrial applications is a big challenge. This work is to investigate the combustion performance of a can combustor using CH_4/NH_3 blended fuels for a micro gas turbine. Results indicated the flame temperature declined with increasing mole fraction of NH_3 at constant fuel flow rates due to a lower heating value of ammonia. To maintain the same power output with increasing NH_3 content, the mass flow rates of the fuel blends need to be raised, which pushed the flame downstream and resulted in severe temperature fluctuation at the combustor exit. The consideration of fuel injection and cooling strategy in the combustor is necessary for future implementation of the fuel blends in this micro gas turbine.

Paper ID: 27

Reaction characteristics of coal/NH_3 co-combustion affected by the highly preheated temperature under mild mode

Zewu Zhang (Huazhong University of Science and Technology), Zhenghong Zhao (Huazhong University of Science and Technology), Liqi Zhang (Huazhong University of Science and Technology), Xiaojian Zha (Huazhong University of Science and Technology)

In this study, the effects of the preheated temperature on coal/NH_3 co-combustion under MILD mode are clarified. Results show that, as the preheated temperature increases, the ignition of coal/NH_3 co-combustion is in advance. The process of coal pyrolysis is earlier to occur, and the consumption of the volatile and NH_3 are accelerated. By contrast, the consumption of NH_3 is prior to that of the volatile. With an increased temperature, the values of *Da* reduce, indicating that the establishment of MILD regimes for coal/NH_3 co-combustion is easier. When the preheated temperature increases from 1173 K to 1923 K, the ignition time is in advance by 21.9%, and the ignition temperature and burnout time are reduced by 26.1% and 22.2%, respectively. In addition, the NOx conversion ratio is increased from 2.78% to 3.25%, which is attributed to the decrease in the proportion of NOx reduction.

Paper ID: 28

Learning combustion state classification from very few IR images using Siamese networks and k nearest neighbors

Kang Ruiyuan (Khalifa University), Panos Liatsis (Khalifa University), Dimitrios C. Kyritsis (Khalifa University)

Current success of machine learning on image-based combustion monitoring is built on massive data, which

is costly even impossible for industrial applications. To address this conflict, we introduce Siamese Network coupled with k Nearest Neighbors (SN-kNN) to combustion monitoring for the first time. In this work, we analyze the training process, test performance and feature visualization of SN-kNN on Infrared (IR) images. The results demonstrate that SN-kNN is capable to distinguish combustion states from learning with merely 20 images per combustion state, the performance on test set is decent with Precision at 0.957, and Accuracy, Recall, and F1-score all at 0.953. Although the feature visualization demonstrates multiple and complex patterns exist inside the class, the mechanism of SN-kNN can eliminate this difficulty and provide robust performance. This work demonstrates the feasibility of using SN-kNN and very few IR images to realize combustion state classification.

Paper ID: 29

Application of latent heat storage system in thermal power plants

Hyo Jae Jeong (Korea Institute of Industrial Technology), Dongho Park (Korea Institute of Industrial Technology), Jong Hyeon Peck (Korea Institute of Industrial Technology), Jae-Hyun Song (SGE Energy Co., Ltd.), Sung Il Kang (SGE Energy Co., Ltd.)

Renewable energy generation is rapidly increasing in the world to minimize the global warming effect. In the Republic of Korea, the renewable energy supply has been accelerated by the 2050 carbon neutral strategy. This present study suggested to ensure operational flexibility by shortening the start-up time of existing thermal power plants to respond the decrease in power reserve due to the rapid expansion of the renewable energy generation ratio. It is possible to store heat during normal operation and release heat during start-up to enhance operation flexibility and reduce greenhouse gas and pollutants generated during start-up by application of the latent heat energy storage system to existing thermal power plants.

Paper ID: 30

Evaluating the rings cleavage mechanism of polycyclic aromatic hydrocarbons in supercritical water: a ReaxFF molecular dynamics study

Hao Zhao (Xi'an Jiaotong University), Yingjia Zhang (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University)

The ring opening reaction of polycyclic aromatic hydrocarbons (PAH) is one of the rate-determining steps in the supercritical water coal gasification process. A series of reactive molecular dynamics simulations were performed to study the ring opening reaction of naphthalene under 2500 K – 2700 K. Species and elementary reactions were extracted from bond orders by an in-house code. Isomers with the same ring structure have been merged to clarify the key reaction paths. The reaction path analysis shows that the ring opening path of naphthalene mainly includes pyrolysis, H atom abstraction, and OH radical addition reaction. The species flux analysis indicates that OH radical is mainly from the reaction of $H + H_2O = OH + H_2$, and the $H_2O = H + OH$ reaction is close to equilibrium, rarely contributing the OH radical. The pyrolysis of naphthalene provides most of the H atom. This atom-level kinetics analysis is prospective to guide the modeling of supercritical water gasification.

Paper ID: 31

Nitrous oxide supported combustion and NO_x formation of counter-flow ethylene diffusion flames

Chun-Wei Huang (Chang Gung University), Dong Chen (Chang Gung University), Hsin-Yi Shih (Chang Gung University), Taro Hirasawa (Chubu University)

The quest for green propellants to replace highly toxic hydrazine (N_2H_4) continues these days. One of the alternatives is nitrous oxide fuel blends (NOFBX). Nitrous oxide (N_2O) can serve as a monopropellant and C_2H_4/N_2O is one of the fuel blends applied in rocket industry because of its high specific impulse. The flame structure and NO_x formation of counter-flow C_2H_4/N_2O diffusion flames were numerically investigated. Results indicated the heat release from N_2O decomposition elevated flame temperature dramatically, and it is mainly from nitrogen based chemistry, especially from $N_2O+H=N_2+OH$ and $N_2O+OH=N_2+HO_2$. In contrast, the heat release of N_2/O_2 supported flame is caused by hydrogen combustion, as strain rate increased, the maximum flame temperature decreased due to reaction of $C_2H_3+M=C_2H_2+H+M$, besides less residence time. In the N_2O supported flame, the key NO formation is N_2O intermediate route ($N_2O+O=2NO$), while the thermal and prompt routes become the NO consumption reactions.

Paper ID: 32

NO emission characteristics of turbulent premixed ammonia-methane flames in a swirl combustor

Yongqian Wang (Jiangsu University), Ping Wang (Jiangsu University), Cheng Kang (Jiangsu University), Weijia Qian (Jiangsu University), Zhengchun Yang (Jiangsu University), Wenfeng Liu (Jiangsu University), Mingmin Chen (Shanghai Electric Gas Turbine Co., Ltd.), Ferrante Antonio (Centro Combustione Ambiente Srl)

In order to study the NO emission characteristics of ammonia/methane turbulent premixed swirling flames, a series of experimental measurements and chemical reactor network (CRN) calculations were carried out. The results show that the flame becomes unstable with the increase of NH_3 mixing ratio. The emission of NO first increases and then decreases with the increase of NH_3 mixing ratio. With the increase of equivalence ratio, the NH_3 mixing ratio corresponding to the NO emission peak in lean combustion increased, while the NH_3 mixing ratio corresponding to rich combustion decreased. With the increase of burner height, NO emission decreases obviously. With the increase of air flow rate, NO emission increases for lean flames but decreases for rich flames. In addition, CRN was used to calculate and analyze the corresponding flame states, and it was found that the predicted NO emission level was not accurate enough, although its overall trend was close to the experimental results.

Paper ID: 33

Skeletal oxidation mechanisms construction and derivation using reaction rate rules: a case study of C_6–C_{14} 1-alkenes

Shuai Huang (Dalian University of Technology), Yachao Chang (Dalian University of Technology), Ming Jia (Dalian University of Technology)

This work presents a novel method for skeletal oxidation mechanism construction and derivation for fuels sharing similar molecular structures using only one referential skeletal model based on the reaction-class-based global sensitivity analysis and reaction rate rules.A case study was conducted on building a set of

skeletal oxidation mechanisms for 1-alkenes from 1-hexene (C_6H_{12}-1) to 1-tetradecene ($C_{14}H_{28}$-1) since olefins are essential intermediates in the combustions of large hydrocarbons and vital precursors of large polycyclic aromatic hydrocarbons and soot. For each 1-alkene, the skeletal mechanism includes ~54 species and ~216 reactions.The skeletal mechanisms were validated against experimental data extensively including laminar flame speeds, ignition delay times, and key species concentrations. Satisfactory prediction performance of all the skeletal mechanisms of 1-alkenes is obtained under wide operating conditions.

Paper ID: 34

Large eddy simulation of ammonia-methane premixed turbulent flames with different wall temperature conditions

Cheng Kang (Jiangsu University), Ping Wang (Jiangsu University), Yongqian Wang (Jiangsu University), Qian jia (Jiangsu University), Yang Chun (Jiangsu University), Antonio Ferrante (Jiangsu University), Chen Min (Shanghai Electric Gas Turbine Co), Liu Feng (Jiangsu University), Roy Subhajit (Jiangsu University)

In this paper, large eddy simulation combined with Dynamic Thickened Flame (DTF) combustion model is used to study the combustion and emission characteristics of NH_3-CH_4, with different wall temperature (700 K, 1150 K, 1500 K, adiabatic) conditions. The results show that a large amount of heat loss weakens the combustion intensity near the wall and even causes local blow off. As the wall temperature decreases, the intensity of HNO and other sources of NO formation decreases, and the amount of NO formation decreases. Comparing the experimental and LES results, it is found that the NO emission at a wall temperature of 1150 K is better. The influence of heat loss must be considered when calculating the NO emission of ammonia fuel combustion. LES can effectively guide the CRN model, and the predicted T and NO trends are the same as those calculated by LES.

Paper ID: 35

Computed NOx emission and flammability of opposed-jet CH_4/NH_3 and H_2 /NH_3 diffusion flames

Yong-Yi Zhuang (Chang Gung University), Yu-Hung Lin (Chang Gung University), Hsin-Yi Shih (Chang Gung University)

The combustion and NO emission of CH_4/NH_3 and H_2/NH_3 blended fuels as alternative energy sources were studied. By using the configuration of opposed-jet diffusion flames, the effects of the NH_3 concentrations on the flame structures, flammability and NO formations of CH_4 and H_2 were investigated and compared. After adding NH_3, the maximum temperature dropped because of the low heating value of NH_3. However, NO net production rate increased with NH_3 concentration but temperature decreased with it, which means that NO emission is dominated by Fuel NO rather than thermal NO. In terms of the highest NH_3 percentage where the diffusion flame cannot exist, H_2/NH_3 fuel blends have wider flammable ranges.

Paper ID: 36

Predicting hybrid vehicle state of charge using time-series based deep learning models

Juan C Giraldo Delgado (KAUST), Inna Gorbatenko (King Abdullah University of Science and Technology), S. Mani Sarathy (KAUST)

Hybrid vehicles are important in achieving a smooth transition to cleaner mobility. Their performance and efficiency are linked to the state of charge (SOC) of the battery, a critical parameter in defining battery performance. An accurate estimation and control of SOC can help in optimizing the performance of the battery and prolong its lifetime. Hybrid vehicle performance can be assessed through analyses of publicly available on-road tests and data-driven algorithms. At the same time, machine learning offers new capabilities in modelling these complex systems in time by learning from data instead of demanding detailed modelling. Here, deep learning models were trained using dynamometer data to provide accurate estimation of SOC during vehicles operation. A recurrent network model using long short-term memory units showed the best performance in predicting SOC. Also, transformer models were effective in modeling vehicle behavior.

Paper ID: 37

A reduced reaction mechanism for an isoparaffinic alcohol-to-jet synthetic paraffinic kerosene (AtJ-SPK)

Jiangkuan Xing (Kyoto University), Zhenhua An (Kyoto University), Yanqi Zhang (Kyoto University), Ryoichi Kurose (Kyoto University)

Alcohol-to-jet Synthetic Paraffinic Kerosene (AtJ-SPK), as one of the approved Sustainable aviation fuels (SAFs), has recently been experimentally studied, and detailed mechanisms have been developed for its oxidization. However, those mechanisms are very huge and hard to be used in Computational Fluid Dynamics. To this end, this paper aims to develop a reduced mechanism for AtJ-SPK from the LLNL detailed mechanism. A reduced mechanism, including 149 species and 732 reactions, could be obtained after the DRGEP, DRGPFA, and FSSA reduction. The reduced mechanism could well reproduce the detailed mechanism predictions on the ignition delays and laminar flame speeds for wide ranges of initial temperatures, pressures, and equivalence ratios. Furthermore, the computational cost of the reduced mechanism only accounted for less than 1/5000 of that of the detailed mechanism.

Paper ID: 38

Effects of Miller cycle combined with supercharging on the performance of a kerosene-fueled pre-chamber jet ignition engine

Fengnian Liu (Tianjin University), Lei Zhou (Tianjin University), Zongkuan Liu (Tianjin University), Changwen Liu (Tianjin University), Haiqiao Wei (Tianjin University)

Kerosene-fueled spark ignition or jet ignition engines have difficulty in knock suppression, which causes deteriorated power and fuel economy. This work introduces the Miller cycle strategy through an electrohydraulic VVT system in a single-cylinder engine to verify the Miller cycle's effects on knock suppression and performance. The result shows that the optimized Miller cycle strategy can help the engine operate with the widely-open throttle with IMEP reaching 7.35 bar, 30.3% larger than the Otto cycle condition. The ISFC of the optimized Miller cycle strategy is 329g/kWh, which is 7.1% lower than the Otto cycle condition. Compared with reducing compression ratio, the Miller cycle strategy can achieve the same power but with better fuel economy. The EIVC60 Miller cycle with 1.6 bar intake pressure has an IMEP of 9.76 bar and an ISFC of 324g/kWh, 12.7 % lower than the low compression supercharging strategy with equivalent power performance.

Paper ID: 39

Lewis number effect for lean premixed H_2-air and CH_4-air flames during combustion instability in a low-swirl combustor

Judai Masugi (Keio University), Takeshi Shoji (Japan Aerospace Exploration Agency), Yoshihiro Nakazumi (Keio University), Ryota Fujii (Keio University), Takuya Tomidokoro (Keio University), Shigeru Tachibana (Japan Aerospace Exploration Agency), Takeshi Yokomori (Keio University)

Combustion instability was observed in both hydrogen and methane flames stabilized in a low-swirl combustor. The pressure fluctuation measurement, OH* chemiluminescence imaging, and PIV were performed simultaneously. By applying the phase-locked averaging method at the flame base, the Lewis number effect was assessed. In the hydrogen flame, since Le < 1, there was a strong correlation between the flame stretch rate fluctuation and the chemiluminescence intensity fluctuation, which indicates that the Lewis number effect is clearly observed. On the other hand, in the methane flame, since Le ≈ 1, there was a weak correlation between the flame stretch rate fluctuation and the chemiluminescence intensity fluctuation, which means the Lewis number effect was not accepted. In the hydrogen flame, the Lewis number effect may be partly responsible for the fluctuation of the heat release rate in the feedback process of combustion instability.

Paper ID: 41

Simulation and experimental study on refuse derived fuel gasification in a downdraft gasifier

Tung Minh Phung (The University of Danang), Tien Minh Nguyen (The University of Danang)

Application of renewable energy to replace fossil fuels is an urgent issue to reduce greenhouse gas emissions, contributing to the implementation of the Net Zero strategy. Vietnam is a tropical country thus biomass is largely abundant. Therefore, gasification of biomass through RDF to produce syngas to power generators is potential for our country. To ensure storage possibility and to improve fuel uniformity, biomass from agricultural waste is processed into RDF. RDF is then gasified to produce syngas to fuel internal combustion engines. This work contributes to the experimental study of gasification of RDF biomass in a downdraft gasifier. The results show that the maximum temperature of the gasifier body ranges from 600°C to 800°C, when the inlet air flow changes from 200L/min to 300L/min. The location of the reaction zone and the maximum temperature zone is independent with the air flow supplied to the gasifier.

Paper ID: 42

Co-oxidation of carbon monoxide and methane under high temperature with monolithic catalyst

Chung-Wei Fu (Industrial Technology Research Institute), Yi-Hsing Lin (Industrial Technology Research Institute), Yu-Lun Lai (Industrial Technology Research Institute)

Four monolithic catalysts, fabricated from $CuMn_2O_4$, $CuAl_2O_4$, $NiAl_2O_4$, and CuCeOx, were prepared for the oxidation of carbon monoxide (CO) and methane (CH_4). Under high temperatures (700-1000°C), the cooperation of the catalysts can enable complete oxidation of CO and CH_4. The CuCeOx catalyst exhibited the best performance compared to the others due to its excellent thermal stability and unique porous structure. After 50 cycles of testing, the conversion of CO and CH_4 remained at higher than 95% and 90%, respectively.

Paper ID: 43

A preliminary study on thermal - mechanical stress of a piston in a heavy-duty diesel engine operating under warming-up conditions.

Nguyen Van Duong (Le Quy Don Technical University), Phuong X. Pham (Le Quy Don Technical University)

Experimental and theoretical studies on engine transient conditions are quite limited in the current literature due to difficulties in (i) setting up experiment and (ii) determining the boundary conditions (BC). This study developed a CFD-FEM model to investigate thermal-mechanical stresses of a piston utilized in a heavy Cl engine under different warming-up conditions. The model was developed with an account for the variations of coolant temperature and element temperature as well as BC. It shows that the piston's thermal-mechanical tresses are significantly varying during warming-up especially in the piston head zone. Variations in the rate of stress and temperature rises are significant. Selecting suitable warming-up procedures may help to improve warming-up quality, piston's and therefore engine's strength and lifetime. This suggests suitable exploitation steps to avoid any critical conditions that may distort/crack/damage the piston or impair its strength/lifetime.

Paper ID: 44

Effect of initial temperature and initial pressure on upper flammability limit of ethylene/air mixtures

Chang Qi (Dalian University of Technology), Ye Ning (Dalian University of Technology), Yalei Wang (Dalian University of Technology), Xingqing Yan (Dalian University of Technology), Jianliang Yu (Dalian University of Technology)

To prevent and control the potential explosion risk of flammable gas mixtures in high-temperature and high-pressure processes, the upper flammability limit of ethylene/air mixtures was tested at initial temperatures of 20-200°C and initial pressures of 0.1-1.5 MPa using self-built 20L spherical explosion characteristic experimental apparatus. The results indicate that the upper flammability limit of ethylene increases with increasing temperature and pressure. The upper flammability limit exhibited an exponential relationship with the initial pressure and a linear relationship with the initial temperature. Additionally, the effect of temperature and pressure synergy on the upper flammability limit was significantly more significant than the sum of the two factors alone, implying that the likelihood of ethylene explosions is higher at high temperatures and pressures.

Paper ID: 45

Simultaneous imaging of nitric oxide and hydroxyl radical with a single laser dye laser in hydrogen jet flames

Karl P. Chatelain (KAUST), Guoqing Wang (King Abdullah University of Science and Technology), Thibault Guiberti (KAUST)

Simultaneous imaging of nitric oxide (NO) and hydroxyl radical (OH) is obtained with the planar laser-induced fluorescence technique by using a single dye laser and two intensified CCD (ICCD) cameras. The technique is demonstrated on two turbulent rich hydrogen-air flames at atmospheric conditions. Several laser excitation wavelengths are employed within the $A^2\Sigma+ - X^2\Pi(0,0)$ and $A^2\Sigma+ - X^2\Pi(1,0)$ vibrational bands of NO and OH, respectively. In this specific configuration, the laser excitation wavelength of each beam is

controlled with a single dye laser's grating angle. As a result, the laser excitation wavelength can be optimized so that: (i) both LIF signals are obtained simultaneously; (ii) the laser excitation wavelength is optimized for OH-PLIF (i.e., near 283 or 284 nm); (iii) the laser excitation wavelength is optimized for NO-PLIF (i.e., 225 and 226 nm). The OH and the NO formation zone are consistent with the different excitation strategies on both flame conditions.

Paper ID: 46

Analysis of dominant reaction mechanism of unstable combustion behavior of ammonia/hydrogen blending system

Mengze Ai (Capital Normal University), Shengyao Liang (Capital Normal University), Lin Ji (Capital Normal University), Dan Zhao (University of Canterbury)

To illustrate the kinetic origin of unstable combustion state in NH_3/H_2 system, their dominant reaction mechanism and corresponding influencing factors are discussed by applying heat release & temperature sensitivity and functional weighting analysis. It is revealed that the major reactions for unstable combustion usually have loop-formed interaction that include both exothermic and endothermic reactions. This creates thermokinetic feedback that promote the reactions with opposite thermal effects kinetically, which drive the system into non-constant oscillatory heat release state. Quantitative standards as well as influencing factors of these thermokinetic driving force are discussed.

Paper ID: 47

The hydrogen generation analysis from dimethyl ether in a novel partial oxidation catalytic fluidized bed reactor using the Kriging surrogate model

Chih-Yung Wu (National Cheng Kung University), Bo-Wei Wang (National Cheng Kung University), Tung-Han Wu (National Cheng Kung University), Shih-Peng Chang (National Cheng Kung University), Shang-Chih Lin (National Cheng Kung University)

The present study intends to present a fluidized bed reactor filled with platinum catalytic beads and quartz sand. It was utilized for syngas generation via partial oxidation of dimethyl ether (DME). By the proposed methodology, the test runs can be reduced by 75.3% to obtain reliable information. The measured experimental results were used as the basis to construct the Kriging surrogate model. In the operation region, the results delineate that the start-up temperature is the most negligible factor in hydrogen generation. Because hydrogen generation was focused, the present study can be regarded as a basis for evaluating the DME as a hydrogen carrier and the proposed novel fluidized bed reactor.

Paper ID: 48

Experimental study on thermoacoustic instability excitation of hydrogen-enriched premixed flame under different swirl numbers

Longjuan Ji (Xi'an Jiaotong University), Weijie Zhang (Xi'an Jiaotong University), Jinhua Wang (Xi'an jiaotong University), Guangya Hu (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University)

Thermoacoustic instability (TI) of hydrogen-enriched lean premixed flame was studied on a swirl and bluff-body burner with different swirl numbers (S=0, 0.42, 0.73). With a constant equivalence ratio Φ, the

experiment was carried out under different inlet velocities U, hydrogen concentration ηH and S. Results show that TI can be triggered by increasing one of these variables without changing the other variables. Besides, S has little effect on the flame oscillation frequency. The OH-PLIF was used to capture the OH profile, and it is confirmed that the triggering of TI is caused by the strong coupling of flame and vorticities. The curvature of the flame front was calculated as an indicator of the flame response to the impact vorticities. When the flame transforms from a stable to a transient or unstable state by increasing ηH at different S, the mean absolute curvature (κabs) of the flame front also increases largely, indicating that TI may be predicted by the κabs of the flame front.

Paper ID: 49

Experimental and modeling study of sewage sludge smoldering combustion at different airflow rates

Wei Zhang (University of Science and Technology of China), Xiaowei Wang (Guangdong Ocean University), Haowen Li (Chinese Academy of Sciences), Zixin Yang (Chinese Academy of Sciences), Qianshi Song (Chinese Academy of Sciences), Xiaohan Wang (Chinese Academy of Sciences)

The objective of this study is to investigate the effects of airflow rate on sewage sludge smoldering combustion by combining experimental and modeling analysis. The experimental results show that the air channeling is easily formed at the reactor's edge, intensifying the reaction and forming a concave smoldering front. As the airflow rate increases, convective heat transfer becomes dominant over conduction and radiation, while the permeability of the fuel increases nonlinearly, resulting in a surge in smoldering propagation velocity (us) and temperature (Tp) at 1 cm/s, followed by a linear increase. The maximum airflow rate at which the smoldering process can propagate stably during sewage sludge disposal is 8 cm/s. The expressions of the smoldering characteristics were obtained by the approach of activation energy asymptotic (AEA), the calculated and experimental values are found to have the same trend of variation, and the agreement is better at low airflow rates.

Paper ID: 50

Overview of shuttling transverse combustion: continuous detonation in a linear wall-bounded channel

Xin Huang (National University of Singapore), Po-Hsiung Chang (National University of Singapore), Zhen Wei Teo (National University of Singapore), Jiun-Ming Li (National University of Singapore), Chiang Juay Teo (National University of Singapore), B. C. Khoo (National University of Singapore)

This study presents our recent research accomplishments for a novel pressure gain combustion combustor that applies the continuous detonations, named shuttling transverse combustion (STC). The concept is to let detonation waves undergoing continuous propagation, reflection and collision in a liner wall- bounded channel, so as to attain the pressure gain combustion. In this study, the detonation wave characteristics of the STC, the identification of reacting zone structures for the continuous detonations in the STC, and the unsteadiness measurements of the STC's exhaust flows were reported. To meet these aims, high-speed flame luminosity imaging, fast-response wall pressure measurements, OH-PLIF imaging technique, OH* chemiluminescence imaging technique and two-dimensional double-frame PIV system were developed and employed.

Paper ID: 51

Effect of copper chromite on ammonium perchlorate decomposition - a TGA-FTIR-MS study

Shani Saha (Indian Institute of Technology Bombay), Arindrajit Chowdhury (Indian Instititute of Technology Bombay), Neeraj R Kumbhakarna (Indian Institute of Technology Bombay)

The effect of copper chromate catalyst ($CrCuO_4$) on the decomposition of ammonium perchlorate (AP) was investigated using thermogravimetric analysis (TGA) combined with Fourier transform infrared (FTIR) spectroscopy and electron ionisation (EI) mass spectrometry (MS) of the evolved gases. To determine the activation energy of AP samples, the Kissinger-Akahira-Sunose iso-conversional method was used, which shed more light on the effect of $CrCuO_4$ on both the low temperature decomposition (LTD) and high temperature decomposition (HTD) stages. The FTIR and mass spectra revealed species O_2, N_2O, Cl_2, NO_2, HCl, HNO_3, H_2O, ClO, HOCl, and m/z = 30. Using $CrCuO_4$, species concentration increment was detected in the HTD stage for all the AP samples. Rise in the ratio of NO_2 to HCl for pellet of mixed AP and $CrCuO_4$ in the LTD stage suggests an accelerated path of NO_2 production. This demonstrates that the presence of $CrCuO_4$ near AP causes ageing, which results in a decrease in burn rate over time.

Paper ID: 52

Combustion of biomedical waste in an oxygen-enriched environment

Abdul Kadir M Poonawala (Indian Institute of Technology Bombay), Shyamal Bhunia (Indian Instititute of Technology Bombay), Neeraj R Kumbhakarna (Indian Institute of Technology Bombay), Arindrajit Chowdhury (Indian Instititute of Technology Bombay)

The Bio-Medical Waste Management (BMW) in India with improper segregation, ineffective combustion, and complacent attitude towards emission control reduces incineration feasibility. The current study focuses on the oxy-enriched combustion of BMW without additional fuel. Selecting the optimum oxygen enrichment value and formulating a composition for the surrogate that best represents the incinerable category of BMW is attempted. Combustion using an experimental setup is used and the combustion characteristics are interpreted for multiple runs using the surrogate. Oxygen enrichment levels varying between 50 to 250 lpm above the baseline oxygen content in primary air were found to be optimum based on the temperature profile inside the incinerator and combustion rate. The surrogate consisted of medical-grade cotton and polypropylene (PPE) representing the yellow category of BMW, excluding anatomical waste and PVC. Multiple experiments with different O_2 levels suggest that higher oxygen lancing near the secondary zone improved the combustion characteristics significantly with less smoke, faster combustion rates, higher peak flame temperature, and uniform combustion of the initial volatiles released while lower levels of enrichment are needed during the gradual release of volatile and char combustion phase.

Paper ID: 53

Temperature and multi-species measurements during $CH_4/H_2/NH_3$ oxidation behind reflected shock waves

Dao Zheng (Tsinghua University), Dong He (University of Science and Technology of China), Yanjun Du (North China Electric Power University), Yanjun Ding (Tsinghua University), Zhimin Peng (Tsinghua University)

Ammonia (NH_3) is considered a promising hydrogen carrier and carbon-free fuel, which can be synthesized using renewable energy. This study simultaneously measured the temperature, CO, CO_2, H_2O, NH_3, and NO time-histories during the oxidation of $CH_4/H_2/NH_3$ mixture (equivalence ratio ≈ 1.2) behind reflected shock waves using laser absorption spectroscopy. Six absorption lines were selected to achieve the measurements. The Glarborg 2018, Sun 2022, and Wang 2022 models were selected to perform detailed analyses in the manuscript. All three models capture the temperature, CO, and H_2O plateaus but overpredict the CO_2 plateau at the near-equilibrium stage. The Glarborg model overpredicts the reactivity, while the Sun and Wang models underpredict the reactivity. The NO plateaus predicted by the Glarborg and Sun model are in good agreement with the measurements. NH_3 and NO were selected as the target species to perform the rate-of-production (ROP) and sensitivity analyses.

Paper ID: 55

Pilot power ratio effect on the structure of turbulent NH_3-CH_4-air swirl flames at atmospheric pressure

Cristian D. Avila Jimenez (KAUST), Thibault Guiberti (KAUST), William Roberts (KAUST)

This work presents an experimental study on the influence of the pilot flame's power ratio on the structure of a turbulent swirling flame. A reduced-scale burner, inspired by that fitted in the AE-T100 micro gas turbine, was implemented as the experimental platform to evaluate an ammonia-methane fuel blend with an ammonia volume fraction of 0.7, with methane as the baseline. The power ratio (PR) between the pilot flame and the main + pilot flame was varied from 0 to 20% for both fuel compositions tested. Qualitative OH-PLIF images of the main flame were recorded to investigate further the effect of the PR on the normalized OH area and flame's front curvature and corrugation factor. Results showed that the OH concentration and the flame structure are significantly modified by the PR for NH_3-CH_4-air flames under the tested conditions. In addition, PR of 10 and 5 % are found to produce more stable flames for CH_4-air and NH_3-CH_4-air, respectively, also characterized by a more corrugated flame front.

Paper ID: 56

Structure of formic acid and n-decane blended counterflow flames

Adamu Alfazazi (King Abdullah University of Science and Technology), Et-touhami Es-sebbar (King Abdullah University of Science and Technology), Jiajun Li (King Abdullah University of Science and Technology), S Xiayuan Zhang, Marwan Abdullah (Saudi Aramco), Mourad Younes (Saudi Aramco), Mani Sarathy (King Abdullah University of Science and Technology), Bassam Dally (King Abdullah University of Science and Technology)

Formic acid (FA) can be produced from renewable hydrogen (H_2) & carbon dioxide (CO_2) and is low in carbon intensity when burned. The objective of this study is to understand the flame behavior of FA/higher hydrocarbon blends. The structure of FA and FA plus n-decane mixtures in the counterflow non-premixed laminar flame configuration were calculated using Chemkin-Pro. Simulation were carried out using Yin et al. FA chemical kinetics model, 2021. The Model was extended to include n-decane sub-chemistry, developed by Sirio and Zhang et al. 2022. Results show that the reactivity of FA can be improved by n-decane substitution. Also, results from kinetic analyses show that HOCO and OCHO are important intermediates for pure FA

flames, reacting with active radicals such as H and OH to produce CO_2 and CO. For n-decane blended flames, most of the fuel decomposition proceeds through H_2 and H_2O abstractions, directly producing CO and CO_2 species.

Paper ID: 57

Numerical simulation of upward bending of horizontal subsonic jet spray flame under sub-atmospheric pressure

Kai Xie (Weifang University of Science and Technology), Yunjing Cui (China University of Petroleum), Xiufeng Tan (Weifang University of Science and Technology)

Combustion and flame utilization in plateau environment are becoming more and more widespread, but the mechanism of its change is not completely clear. The purpose of this paper is to reveal the combustion mechanism and flame bending characteristics of horizontal spray flame under sub-atmospheric pressure. Based on the discrete phase (DPM) random trajectory model, large eddy simulation (LES) and probability density function (PDF) are used to calculate the horizontal spray flame with rated air volume flow rate, and the results were compared with the previous experiments. The combustion mechanism of the flame is analyzed from the perspective of component change. The density distribution can better reveal the morphologic mechanism of the flame region of the buoyancy plume. The dimensionless density at the terminal flame section is negatively correlated with the natural logarithm of atmospheric pressure.

Paper ID: 59

Numerical simulation of solid fuel ramjet combustion with regression model

Wen-Hsuan Liang (National Chung-Shan Institute of Science and Technology)

The complexity of solid fuel ramjet (SFRJ) combustion originates from mutual coupling factors regarding diffusion flow in the air intake, flow recirculation zone in the combustor entrance, reattachment in the fuel port, as well as expansion flow in the nozzle. Furthermore, regression rate of the solid fuel is affected by the inlet air total temperature, mass flow rate, combustion chamber and fuel grain geometry. Numerical simulation of SFRJ combustor flow field was performed and the influences of inlet air conditions and combustor pressure on fuel regression rate characteristic were analyzed. Results show that fuel regression rate is dependent of inlet air total temperature and mass flow rate, but not on chamber pressure.

Paper ID: 61

Simulation of ignition process in a solid rocket motor with jettisoned ignitor

Wen Jing Wu (NCSIST)

Simplified physical models and numerical methods were presented to simulate the ignition process in a solid rocket motor with jettisoned ignitor. Two typical test data with and without link block behind the ignitor were used to validate the model parameters. The discrepancy between simulation and measurement is reasonable for these two cases. The quicker pressure rising rate for the case with link block can be attributed to relative slower jettison of ignitor and higher flame spreading speed on propellant surface. Finally, the predicted higher pressure peaks with increasing ignitor release force within our range might cause insignificant effects if a reasonable safety factor design has been considered.

Paper ID: 62

Dynamic response of lean premixed swirl flames to nanosecond repetitively pulsed discharges at pressures up to 2 bar

Liang Yu (King Abdullah University of Science and Technology), Aravind Balakrishnan (King Abdullah University of Science and Technology), Deanna Lacoste (King Abdullah University of Science and Technology)

The response of premixed swirl methane-air flames to acoustic forcing with and without nanosecond repetitively pulsed (NRP) discharges is investigated in this study. Experiments were carried out at two pressures of 1.2 and 2.0 bar, with equivalence ratios of 0.79 and 0.75, respectively. The applied voltage was 5.0 kV at 1.2 bar and 6.2 kV at 2.0 bar, with a constant pulse repetition frequency of 70 kHz. A loudspeaker was used to force the incoming flow, with an amplitude of 10% of the bulk flow velocity. Fluctuations of heat release rate were measured by phase-locked imaging of CH* chemiluminescence using an intensified charge-coupled device camera. Flame transfer functions were then determined and compared. It was found that the NRP discharge affected the flame transfer function by reducing the gain in the range of frequencies 64 to 208 Hz, while barely affecting the phase. Two mechanisms responsible for the decrease in gain are proposed and discussed.

Paper ID: 63

Experimental investigation of the global characteristics of ammonia spray

Santiago Cardona Vargas (KAUST), Felipe Campuzano Diosa (KAUST), William Roberts (KAUST), Thibault Guiberti (KAUST)

Ammonia has a privileged position as a potential enabler of a low-carbon economy; it is a carbon-free fuel with a high hydrogen capacity (17.8 wt.%) and well-established production and distribution infrastructures, making it a viable option for a zero-carbon energy source. However, ammonia has drawbacks as a fuel that must be addressed. This work aims to experimentally investigate the effect of the boundary conditions (i.e., co-flow and atomizing flow) on ammonia spray dynamics injected by a commercial injector at 0.7 MPa in a confined burner at room pressure and temperature using a backlight imaging technique to clarify ammonia spray features. The results showed that increasing the co-flow and atomizing flow enhances the ammonia atomization quality. Additionally, conditions that promoted unstable ammonia spray formation were observed. The findings of this research will serve as a starting point for the clean and efficient use of ammonia as a fuel in combustion-based technologies.

Paper ID: 64

Experimental study of 2-methylbutanol autoignition

Ruozhou Fang (University of Connecticut), Chih-Jen Sung (University of Connecticut)

Continuing the efforts to provide experimental datasets for model development and validation of the major components of fusel alcohol blends, rapid compression machine (RCM) experiments of 2-methylbutanol (2-MB) in air are conducted herein at varying pressures, temperatures, and equivalence ratios. For the conditions investigated, RCM results show that the total ignition delay time of 2-MB monotonically decreases with

increasing temperature/pressure/equivalence ratio. Although 2-MB exhibits only single-stage ignition behavior in the present RCM experiments, the slope variation on the Arrhenius plots is observed, signifying the changes in controlling chemistry within different temperature ranges. In addition, the present RCM results are compared with the literature shock tube data, and the effects of pressure and equivalence ratio on autoignition of 2-MB are discussed. Furthermore, the comparison of the RCM results of 2-MB and 2-phenylethanol provides insights into the molecular structure effects on chemical kinetics under engine-relevant conditions.

Paper ID: 65

Experimental investigation on plasma-assisted spray combustion of methanol/water mixtures

Hai-Hua Chen (National Cheng Kung University), Xiang-Xin Chen (National Cheng Kung University), Chih-Yung Wu (National Cheng Kung University)

This paper presents the effect of gliding arc discharge on the flame stability of methanol diffusion combustion with different water content was investigated through experiments. The dehydration process is the most energy-intensive step in methanol production. Therefore, this thesis investigated the phenomenon of flame behaviors such as the flame length and lift-off height show that plasma positively affects combustion enhancement. The flame length decreased as the water content in the methanol increased with or without gliding arc plasma assisted. On the contrary, the lift-off height without plasma-assisted increases with water content; the lift-off height with plasma-assisted isn't over 50mm from the nozzle, indicating that plasma enhance combustion stability. According to the distribution of CH* radicals, it was discovered that plasma increases the flame heat release rate, which may be one of the reasons why the flammability limits of water content in methanol was extended.

Paper ID: 66

Investigation on Pd/C catalyzed hydrogenolysis of lignin and its model compound via flow-through reactor coupling ultra-high resolution mass spectrometry

Linyu Zhu (Shanghai Jiao Tong University), Cunhao Cui (Shanghai Jiao Tong University), Jing Zhang (Shanghai Jiao Tong University), Xintong Xiao (Shanghai Jiao Tong University), Haoran Liu (ShanghaiJiaotong University), Zhongyue Zhou (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University)

The irreversible condensation of reactive depolymerization intermediates is one of the foremost obstacles to increasing the monomer yield for lignin utilization. Recently, flow-through reactors have been applied to investigate the behavior of catalytic conversion of lignin. Herein, we coupled a flow-through system with ultra-high resolution mass spectrometry through capillary sampling and six-port valve injection, and realized higher time-resolved analysis with virtually no disturbance to the reaction. Pd/C catalyzed hydrogenolysis of lignin and its model compound was studied by this method, and a molecular-level analysis of product distribution was achieved, which helps to deepen the mechanism insights into the β-O-4 cleavage under late transition metal-catalysis, and demonstrates the marvelous effect of inhibiting condensation by substitution of a batch reactor with a flow-through reactor

Paper ID: 67

Effect of metal-modified ZSM-5 catalysts on lignin pyrolysis properties and aromatic selectivity

Yang Shen (Shanghai Jiao Tong University), Haoran Liu (ShanghaiJiaotong University), Zhongyue Zhou (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University)

The efficient and directional production of aromatic hydrocarbons from lignin is still a scientific problem to be solved. The core problem of lignin to aromatics is the development of selectivity, efficient, low-energy, and low-cost processes of lignin catalytic pyrolysis. Herein Cu2O/HZSM-5 catalysts were prepared and catalyzed kraft lignin-derived pyrolytic vapors to selective production of benzene. On-line photoionization time-of-flight mass spectrometry (PI TOF-MS) experiments were performed to determine the effects of several factors on selective benzene production, including Cu2O loading on HZSM-5, carrier gas flow rate and pyrolysis temperature. Under the optimal conditions, the yield of benzene from the pyrolysis of kraft lignin over Cu2O/HZSM-5 is up to 43.1 mg/g based on dry lignin while those from HZSM-5 catalyst were only 17.2 mg/g.

Paper ID: 68

Study of powder-CH_4-air "hybrid" flames in a stagnation-point flow

Ryoki Okada (Toyohashi University of Technology), Haruya Yata (Toyohashi University of Technology), Daiki Matsugi (Toyohashi University of Technology), Takuya Yamazaki (Toyohashi University of Technology), Yuji Nakamura (Toyohashi University of Technology)

The dynamic response of methane–air premixed flame combined with fine organic powder at the prescribed rate formed in the stagnation-point flow has been experimentally studied. Powder loading device and the burner system are newly developed, and the stagnation-point flow is induced using the spherical obstacles in the premixed flow over the burner. The equivalence ratio of the methane–air mixture is fixed at 0.65, whereas the amount of the loaded powder is varied as a main experimental parameter. The fuel in the present study is a mixture of combustible gas (methane) and solid (biomass). Thus, this study aimed to investigate the fundamental features of a "hybrid" combustion system. Dynamic behavior is taken by a high-speed camera to understand the mechanism of this hybrid system. Initially, the premixed flame is steadily formed in the stagnation flow field. Once the powder is loaded, the flame front moved upwardly and then remained at a certain distance away from the original position or all the way down to attach to the burner surface. The propagation velocity of the hybrid fuel is intensified with the powder. Notably, a critical loading rate to promote the propagation rate is available. High-speed imaging facilitates the investigation of the powder–flame interaction. Although numerous issues must be further improved a conceptual design to study hybrid combustion utilization of stagnation-point flow is ensured.

Paper ID: 69

Experimental study of the flame propagation in the porous media for hydrogen-ammonia premixed fuels

Chien-Ru Yu (National Cheng Kung University), Juan Cerverka (Universitat Politècnica de València), Tien-Chiu Hsu (National Cheng Kung University), Chih-Yung Wu (National Cheng Kung University)

The flame propagation of ammonia blended with hydrogen in the porous media is experimentally evaluated

in the present study. It has been well known that ammonia/air mixtures' laminar flame speed is relatively low. In order to promote and maintain the flame stability, adding traditional fuels is a feasible method. Besides, due to the porous media's intrinsic properties, the heat transfer and heat recovery phenomena can be enhanced to make combustion more stable. In the current research, the theoretical analysis combined with the modified Péclet number and Lewis number was used to estimate whether ammonia-hydrogen flame propagates in the porous media, and verifies it through experiments.

Paper ID: 70

A study of co-gasification of shiitake substrate and PE using ASPEN Plus

Yun-Ting Hsu (National Cheng Kung University), Guan-Bang Chen (National Cheng Kung University), Fang-Hsien Wu (National Cheng Kung University), Ta-Hui Lin (National Cheng Kung University)

The study simulates the co-gasification process of shiitake substrate and polyethene (PE) by using ASPEN Plus. The proposed model used kinetic model with considering tar cracking reactions. The model is then validated by 16 experiments. The validation results - R^2 of CO, CO_2 and H_2 is above 0.8. Furthermore, the influences of gasifying agent, biomass/plastic blending ratio and the gasifier temperature on syngas component are investigated. Adding PE will cause CO and CO_2 decrease due to the lack of oxygen in PE. Also, PE contains higher VM and lower FC leads to the higher production of H_2 and CH_4. Additionally, the CO_2 will decrease with the $CO_2/(H_2O+CO_2)$ increasing, which is in good agreement with Le Chatelier's principle. Finally, CO and CH_4 will enhance with the rising of temperature, while CO_2 and H_2 are decreased. The change by the temperature can be explained by the enhancement of endothermic reactions and tar cracking.

Paper ID: 72

Effect of ammonia enriched gaseous co-flow on soot formation in droplet combustion

Atul Kumar (Natioanl Formosa University), Shouyin Yang (Natioanl Formosa University)

There is increasing interest in using ammonia (NH_3) as a combustion fuel due to its low carbon dioxide emissions. This study investigated the effect of injecting different concentrations of ammonia on soot production during fuel combustion. The results showed that up to 10% ammonia, the diffusion flame was stable, but at 15% ammonia, a dual flame occurred with a diffusion flame at the center and an ammonia flame surrounding it. This is due to the flammability of ammonia, which ranges from 14.8% to 33.5% in air. The dual flame led to hydro dynamic instability and increased the flame length and diffusion area due to the buoyancy effect caused by the enrichment of hydrogen through ammonia decomposition. However, the droplet did not ignite with more than 15% ammonia injection, as the ammonia flame and diffusion became dominant. The soot production rate was effectively lowered with the injection of ammonia from 5% to 15% for all fuels due to the hydrogen enrichment through ammonia.

Paper ID: 74

A study of waste shiitake substrate co-gasification with waste polyethylene

Chung yu Chang (National Cheng Kung University), Guan-Bang Chen (National Cheng Kung University), Fang-Hsien Wu (National Cheng Kung University), Fu-Yuan Yuan (National Cheng Kung University)

As one of the primary agricultural wastes in Taiwan recently, landfill and compost are the main methods to

deal with the waste shiitake substrate. A more efficient way for the environment is required because of the limited land space and the pollution from the over-landfill In this study, a 1KWth-level bubbling fluidized gasifier was used as a reactor. And waste shiitake substrate and waste PE were used as feedstock for the co-gasification experiment. TGA-FTIR was used to analyze the thermal degradation process and the gas production. Meanwhile, activation energy was also calculated. In this study, The Taguchi method was used to find the optimal operating parameters (gasification temperature, blending ratio, $CO_2/(CO_2+H_2O)$, catalyst). The results show that the waste shiitake substrate has a Boudouard reaction at 750°C, and the activation energy is the lowest when the blending ratio is 20%. Water vapor can increase the concentration of H_2. High temperature can increase the CGE.

Paper ID: 75

Experimental study on ignition of the liquid hydrocarbon fuel in a supersonic flow

Po-Kai Chuang (NCSIST)

This article presents the experimental investigation of JP-5-fueled supersonic combustion in direct-connected wind tunnel. The test model is designed with a rectangular cross-section, and there are two cavity flameholders in the combustor. In the test, the hydrogen/air torch igniters were used to ignite JP-5. Various inflow total temperature, hydrogen/air torch igniter energy and number of wall injectors were tested, and the condition to achieve self-sustained combustion of JP-5 was determined. The results show that successful self-sustained combustion occurred as long as the inflow total temperature was above 1500K and the hydrogen/air torch igniters operated at 62kW for 2 seconds. But at conditions where the inflow total temperature was below 1500K, the combustion could not be sustained and even went out immediately after the hydrogen/air torch igniters turned off. That means if the vehicle's engine is designed in this configuration, the inflow total temperature of the engine should not be too low, that is, the engine could not operate at low flight speed. In order to let the engine operate at lower inflow total temperature or flight speed, further study of different configurations is required, such as changing the design of the injector, cavity, etc.

Paper ID: 77

Propagation of nonpremixed methane-air lifted flame in the parallel electric field

Jinwoo Son (KAUST), Min Suk Cha (KAUST), Sunho Park (KAUST)

The effect of electric fields on flames has been studied for centuries, but only recently have numerical studies been conducted. Our previous study experimentally found that the edge flame propagated toward the high-voltage electrode regardless of the applied voltage. To investigate the effect of the electric field on a propagating edge flame in detail, this study developed a numerical code that simulates the electric field on the reacting flow fields. The numerical results, such as flame propagation behavior, velocity field, etc., were compared with the experimental measurements and showed a consistent trend between the simulation and the experiment.

Paper ID: 78

Nanothermite assembly on copper wire mesh blanketed with CuO nanowires via electrophoretic deposition of aluminum nanoparticles

Wan-Lien Hsu (National Cheng Kung University), Ming-Hsun Wu (National Cheng Kung University), Chia-Ting Lin (National Chung-Shan Institute of Technology)

Aluminum particles were electrophoretically deposited on a copper mesh with CuO nanowires grown on the wire surface to form a nanothermite layer. By replacing wire with mesh for the copper substrate, the quantity of nanothermite obtained from each batch becomes not only larger, but also easily scalable. Mesh size, which affects both the mesh wire diameter and the spacing between wires, affects properties of the assembled thermite. The parameters further influence the burn rate of the energetic material. The study first verifies the feasibility of nanothermite assembly on a copper mesh using electrophoretic deposition. The effect of the mesh size on the burn rate of the Al/CuO nanothermite mesh were then experimentally investigated. Commercial copper grids with sizes of 100, 150, 200 and 250-mesh were studied. The deposited mass of aluminum nanoparticles was controlled via the applied deposition duration such that the overall equivalence ratio of aluminum and copper oxides for each case was close to stoichiometric for burn rate comparison. The test results showed that self-sustained reaction propagations were achieved on nanothermites on all meshes. The burn rate along the 250-mesh copper mesh was the fastest, and the reaction was the most intense. It is found that the burn rate increases almost linearly with mesh size.

Paper ID: 79

A volume of fluid approach to model vacuum residue injection in an entrained flow gasifier

Alberto Ceschin (King Abdullah University of Science and Technology), Francisco Hernandez Pérez (KAUST), Hong G. Im (KAUST)

Liquid gasification is often performed in entrained-flow gasifiers: a spray is injected from the top into an oxidizing environment in these reactors. One of the significant challenges of gasification of a liquid feed is to achieve adequate atomization, which results in increased yield of the process and minimization of solid residue formation. In this context, it is crucial to model the injection process. The fuels processed in gasification reactors consist of heavy and generally viscous mixtures. The peculiar physical properties of those fuels need to be adequately modelled in CFD simulations of the injection. This work demonstrates the application of the volume of fluid (VoF) method to simulate injection in an entrained-flow gasifier. The software adopted for the simulations is based on the OpenFOAM library. The liquid volume fraction is advected geometrically using the isoAdvector algorithm with piecewise linear interface construction (PLIC) to resolve ligaments down to tiny droplets accurately. The latter is essential for accurate curvature estimation. Adaptive grid refinement (AGR) helps with this purpose. Also, a transition of smaller droplets to Lagrangian particles unlocks large-scale simulations while optimizing computational cost.

Paper ID: 80

Study of “inverse” droplet combustion using 90 wt. % H_2O_2

Daiki Matsugi (Toyohashi University of Technology), Takuya Yamazaki (Toyohashi University of Technology), Tsuneyoshi Matsuoka (Toyohashi University of Technology), Yuji Nakamura (Toyohashi University of Technology)

Fundamentals of combustion of a single droplet of 90 wt. % H_2O_2 (oxidizer droplet) suspended in a quiescent N_2-balanced CH_4 environment, called “inverse droplet combustion”, were investigated under various ambient

CH_4 concentrations at standard condition (298 K and 0.1 MPa in absolute). Burning behavior of the droplet was recorded, and flame diameter and droplet diameter changed in time were carefully analyzed. Following spontaneous ignition induced by electrically heated wire, a spherical-like flame was successfully established under normal gravity condition, and it was found that the entire burning behavior was exactly same as a normal (fuel) droplet combustion following the classical d-square law. As compared with the normal droplet combustions, the burning rate constant showed faster, and the standoff ratio became smaller, irrespective of the adopted CH_4 concentration. These were mainly attributed to a fact that location of diffusion flame, which was defined by the oxidizer-fuel stoichiometry, shall be closer to the droplet in the present "inversed" case. Alternatively, the potential flame structure was predicted numerically to extract its unique burning characters of H_2O_2 droplet in the CH_4-fueled atmosphere.

Paper ID: 81

Design and test to a high temperature reheater by hydrogen combustion

Fu-Chou Hsiao (NCSIST), Fu-Chou Hsiao (NCSIST), Jing-Yuan Zhou (NCSIST), Jing-Yuan Zhou (National Chung-Shan Institute of Science & Technology)

In our lab, an existing test facility(HTTF) has the test capability of only a lower mass flow rate(main flow) with high temperature(1600K). To satisfy the newly required test flow condition of increased flow rate, a reheater was designed and manufactured to assemble with HTTF. Additional air was introduced to supplement the main flow through the reheater by hydrogen combustion. The hydrogen is autoignited by the high temperature main air flow from HTTF. The key design of the reheater includes the arrangement among the injection of hydrogen, additional air, oxygen, and layout of the water jacket. CFD results verified the design of the reheater before manufacturing and revealed the injections contribute to the flow mixing. The recirculation flows formed by the mixing injections constrain the flame zone away from the inner wall downstream the reheater, which prevents the reheater from high temperature damage. After the reheater assembled with HTTF and all injection flow rates being calibrated, the whole facility test results validated the hydrogen autoignition and the required high temperature flow conditions. Consequently, the test capability of HTTF was successfully augmented by the reheater.

Paper ID: 82

CFD evaluation of NH_3 cofiring with pulverized coal in a commercial tangential-firing boiler

Yunha Koo (Sungkyunkwan University), Hyunbin Jo (Sungkyunkwan University), Seonkyo Ha (Sungkyunkwan University), Woosuk Kang (Sungkyunkwan University), Jongmin Park (Sungkyunkwan University), Sangbin Park (KEPCO Research Institute), Jongmin Lee (KEPCO Research Institute), Sehyun Baek (KEPCO Research Institute), Changkook Ryu (Sungkyunkwan University)

In coal-fired power plants, cofiring NH_3 has emerged as a new strategy to reduce CO_2 emissions. The ideal method for NH_3 cofiring requires to minimize the NOx emission while achieving similar boiler performance in terms of flame stability, combustion efficiency, and heat distribution. In this study, different NH_3 cofiring methods were evaluated in the commercial 500 MWe tangential-firing boiler using computational fluid dynamics. The location of NH_3 injection was varied between different ports across the burner zone. To suppress the fuel NO formation, the burner zone stoichiometric ratio was kept low by increasing the air supply

to the separated over-fire air while the overall excess air ratio was fixed at 15%. It was found that the NOx emission at the boiler exit greatly depends on the location of NH_3 injection and local reaction stoichiometry. Injecting NH_3 at the lowermost burner can be an effective way to keep the NOx emission at a similar level to that for coal combustion only. However, the distribution of secondary air and the injection speed of NH_3 require further optimization to increase heat absorption on the furnace while suppressing the NO formation.

Paper ID: 83

Numerical study on chemical behavior of thermal decomposition of methane under high temperature condition

Sojeong An (Yonsei University), Jinje Park (Korea Institute of Industrial Technology), Youn-sang Bae (Yonsei University), Youngjae Lee (Korea Institute of Industrial Technology)

This study aimed to analyze the chemical behavior of hydrogen production from methane by the thermal decomposition, called turquoise hydrogen, through a numerical approach. PSR and PFR models were used for the reaction analysis. And the calculation was performed using the detailed chemical mechanism consisting of 77 species and 243 reactions. The conversion rate of CH_4 and selectivity of H_2 were predicted in terms of various temperatures, pressures, and residence times. Hydrocarbons showing various concentrations according to the conversion rate of methane were also analyzed. Methane started to decompose above 600 K under equilibrium conditions, and the conversion of CH_4 decreased as the pressure increased in the PSR model. The results of using the PFR model showed that the gas temperature is slowly increased by an endothermic reaction.

Paper ID: 85

The flame height measurements of inverse diffusion methane flames under various conditions: reactant flowrates and oxygen concentration

Carson Chu (KAUST), Ibrahim Alsheikh (KAUST), Peng liu (KAUST), William Roberts (KAUST)

Autothermal reforming (ATR) is a promising technology to economically mass-produce hydrogen, which is seen as a key energy source in the future decarbonized society, from methane. However, ATR is susceptible to catalyst poisoning that is caused by soot formation in the process, subsequently reducing the production yield. How soot forms within ATR, which uses the inverse diffusion flame (IDF) configuration, is unclear. To understand the formation process, a fundamental understanding of IDFs is required. Flame length is an important characteristic of IDFs, as it is used to validate numerical models and to calculate the residence times of soot particles. In this work, the flame lengths were determined by OH* chemiluminescene. The effects of fuel, diluent, and oxidizer flowrates, and oxygen concentration on flame heights were assessed. Flame heights of methane IDFs were reported and it is found that the flame length is governed by the oxidizer flowrate but is affected moderately by the fuel and diluent flow rates. In contrast, flame heights were insensitive to the change in oxygen concentration. The Roper's correlation was used to analytically model the flame length. To accurately predict the flame lengths, the diffusion coefficient and the characteristic flame temperature should be carefully chosen.

Paper ID: 86

Towards accurate simulation on a three-dimensional turbulent partially premixed flame with detailed chemistry and radiative heat transfer

Yang Yinan (Osaka University), Bai Zhiren (Osaka University), Hori Tsukasa (Osaka University), Sawada Shinya (Osaka University), Akamatsu Fumiteru (Osaka University)

The modeling of turbulent reacting flows is complicated since it deals with the description of complex interactions between turbulent transport processes and chemical reactions. A standard experiment with reliable data is therefore necessary to validate the accuracy of the developed turbulent combustion model. In this study, the effect of thermal radiation and grid resolution was discussed through the RANS methodology, based on a partially premixed piloted methane-air jet flame, and was validated by the 2-D structured grids and the 3-D unstructured meshes respectively. The radiative transfer equation is solved using the discrete ordinates method in the conservative finite-volume formulation. On the profiles of centerline species distribution, results show that the inclusion of the radiation model leads to a decrease in the peak temperature but does not significantly influence the flow velocity and mixing fields. The influence of the radiation model mainly occurs at the flame front to the temperature distribution. However, the deviations of major species mass fractions and normalized velocity calculations remain smaller than 5%. Good agreements with experimental results can be reproduced when the minimum mesh size is refined to 0.3 mm. The developed turbulence combustion model has been validated and can be implemented in subsequent methane-ammonia-related industrial combustion scenarios.

Paper ID: 87

A study of building fire safety performance under smoldering

Wai Kit Cheung (The Hong Kong Polytechnic University), Xinyan Huang (The Hong Kong Polytechnic University), Yanfu Zeng (The Hong Kong Polytechnic Univerisity), Shaorun Lin (The Hong Kong Polytechnic University)

Smoldering produces massive toxic smoke and carbon monoxide (CO) that is responsible the majority of fire deaths, but current building fire safety design rarely considers smoldering hazards. This work investigates the transport and hazards of CO from smoldering fire for the building performance-based design practice. The numerical model is firstly validated by reproducing two flat-scale fire experiments, revealing the characteristic surface temperature and CO yield of smoldering sources. The smoldering fire scenario is then designed in an atrium to review the evolution of CO concentration and its associated Available Safe Egress Time (ASET). Results show that a smoldering fire of the same burning rate as a flaming fire can provide a similar ASET. Hence, the smoldering fire scenarios and their CO hazards should be considered in the performance-based design of building fire safety.

Paper ID: 88

A computational study of a laminar methane-air flame assisted by nanosecond repetitively pulsed discharges

Xiao Shao (King Abdullah University of Science and Technology), Narjisse Kabbaj (KAUST), Deanna Lacoste (KAUST), Hong G. Im (KAUST)

Nanosecond repetitively pulsed (NRP) discharges are a promising technique to enhance combustion efficiency

and control. Numerical studies are essential to improve the understanding of complex plasma-combustion interaction. Limited by the prohibitive computational cost of fully coupled detailed plasma mechanism and combustion chemistry, a phenomenological model taken from literature is incorporated into reactingFoam solver in OpenFOAM to study the behavior of a laminar methane-air flame under NRP discharges. The phenomenological model focuses on two channels through which the electric energy is deposited: 1) the ultrafast heating and ultrafast dissociation of O_2 coming from the relaxation of electronically excited N_2; and 2) the slow gas heating coming from the relaxation of vibrational states of N_2. These three coupled plasma enhancement pathways are numerically split by depositing all energy into single ones to investigate their individual roles. The model is applied to an experimental configuration where a lean wall stabilized methane-air flame is actuated by NRP discharges across the flame front. Flame displacement, flame power response, and key radicals' distribution under plasma are qualitatively compared with experimental results.

Paper ID: 89

Numerical modeling of afterburner combustion at two operating conditions

Ching-Chi Wu (National Chung-Shan Institute of Science and Technology)

Afterburners should be functional within a wide range of operating conditions. In order to understand the details of the flow field and combustion characteristics of reacting flow inside an afterburner, computational fluid dynamics techniques are employed. Two operating conditions are investigated, i.e., ground running at sea level and cruising condition at 2.5 Mach and 15 Km. Performance is evaluated by the variation of oxygen and fuel vapor concentration, total pressure loss, Mach number, and total temperature. Fuel is found to be partially unburned during the combustion process, indicating that fuel distribution can be improved. Coolant admitted into the core flow through small holes in the liner produces essential film cooling layer and increases oxygen concentration, however, the increase of flow velocity and the decrease of temperature might reduce the chemical kinetic rates. Therefore, the distribution of mass flow rate is crucial. The numerical modeling of afterburner provides details of the flow and combustion characteristics, which is essential in the design of efficient afterburners.

Paper ID: 90

Elucidating the mechanism for the oxidative coupling of methane catalyzed by La_2O_3: experimental and microkinetic modeling studies

Zaili Xiong (Shanghai Jiao Tong University), Jijun Guo (Shanghai Jiao Tong University), Yuwen Deng (SJTU), Bingzhi Liu (University of Science and Technology of China), Hao Lou (University of Science and Technology of China), Meirong Zeng (Shanghai Jiao Tong University), Zhandong Wang (University of Science and Technology of China), Zhongyue Zhou (Shanghai Jiao Tong University), Wenhao Yuan (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University)

Oxidation coupling of methane (OCM) catalyzed by La_2O_3 was carried out in a packed bed reactor at low pressure conditions over a wide temperature range. Dozens of species, including radicals and stable species like methyl, methoxy and vinyloxy were observed by using synchrotron vacuum ultraviolet photoionization mass spectrometry (SVUV-PIMS). Many of detected species were reported for the first time in OCM reactions. A microkinetic model was developed and validated against the experimental results. The simulation results of

the kinetic model agreed well with the experimental measurements. Reaction pathway and sensitivity analysis revealed the complex reaction network and key reactions of OCM.

Paper ID: 92

Exploration of the optimal ignition position in a model gas turbine combustor

Xiaoyang Guo (Xi'an Jiaotong University), Bowen Liu (Xi'an Jiaotong University), Yunyang Liu (Xi'an Jiaotong University), Erjiang Hu (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University)

Ignition experiments at different discharge positions were conducted in a simplified gas turbine combustor to explore the optimal ignition position. The flow field and spray distribution were clarified by CFD simulation and non-intrusive laser diagnostic, respectively. High-speed CH* chemiluminescence images were used to analyze the ignition process. The normalized CH* chemiluminescence intensity over time indicates that the conventional flame propagation stage and flame stabilization stage can be reclassified into four phases, including rapid kernel propagation stage, wall-attached fuel consumption stage, flame morphology transformation stage, and flame morphology stabilization stage. Statistical analysis of the duration of rapid kernel propagation stage shows that the kernel in the inner recirculation zone is the most favorable for the fast development to a full-flame. The optimal ignition position near the wall should correspond to the widest part of the inner recirculation zone.

Paper ID: 93

Highlights on the mechanism of jet development, flame propagation, and combustion regime in a pre-chamber engine

Mickael Silva (KAUST)

Towards fundamental understanding of the governing physics of flame propagation in pre-chamber combustion, computational fluid dynamics was utilized to compare the relative contribution of convection and turbulent flame propagation in an engine operated with methane. The pre-chamber lodges the spark plug and fuel injector, thus allowing for separate fueling from the main chamber. The combustion is modeled with the G-Equation; the laminar flame speed was obtained from a lookup table generated from a reduced methane oxidation mechanism of the AramcoMech 1.3, while the turbulent flame speed was computed using the Peters' relation. A homogeneous charge of methane is considered with global $\lambda = 1.8$ and 7% of the total fuel added through the pre-chamber. The results show that the strong turbulence generated by the jet is mostly constrained behind the flame (within the jet), and the convection generated by the jet is mostly responsible for the jet/flame development; this is confirmed by comparing the trends of flame area evolution and flow velocity behind the flame. Furthermore, the results reveal a sizable variation of Damköhler values across the flame, for which the median seems to be more appropriate than the mean for classifying the combustion regime according to the Borghi-Peters diagram.

Paper ID: 94

Exploring the influence of no addition to the oxidation of *n*-butanal at low to intermediate temperature: experimental and kinetic modeling

Yuwen Deng (SJTU), Jijun Guo (Shanghai Jiao Tong University), Zaili Xiong (Shanghai Jiao Tong

University), Wenhao Yuan (Shanghai Jiao Tong University), Meirong Zeng (Shanghai Jiao Tong University), Zhongyue Zhou (Shanghai Jiao Tong University), Jiuzhong Yang (University of Science and Technology of China), Fei Qi (Shanghai Jiao Tong University)

The oxidation of pure *n*-butanal and *n*-butanal/NO mixture was investigated in an atmospheric jet stirred reactor at stoichiometric conditions and over the temperature range 425-925 K. Speciation data were obtained by using synchrotron vacuum ultraviolet photoionization mass spectrometry. A submechanism of *n*-butanal/NO_x was developed to interpret the interaction kinetics of *n*-butanal and oxidation intermediates with NO_x species. Experiments revealed that *n*-butanal oxidation was inhibited by NO_x addition in the low temperature regime (< 625 K) while significantly promoted at intermediate temperatures (> 700 K). Besides, the NTC behavior inherent in *n*-butanal oxidation disappeared following the doping of NO_x. The kinetic modeling analyses indicated that in the presence of NO the aldehydic H-atom elimination and the decarbonylation channels of *n*-butanal consumption are significantly promoted. Meanwhile, the low temperature chain-branching steps occurring on the alkyl chain of *n*-butanal are inhibited. This is the leading cause of the decreased reactivity upon NO addition at low temperatures. However, the accelerated NO/NO_2 interconversion kinetics was responsible for the increase in fuel reactivity within the intermediate temperature region.

Paper ID: 95

Influence of a coaxial plasma actuator on the flame stabilization of non-premixed jet flames

Jun-Lin Chen (National Yang Ming Chiao Tung University), Chiang Fu (National Yang Ming Chiao Tung University), Ying-Hao Liao (National Yang Ming Chiao Tung University)

This study is to experimentally investigate the influence of an annular plasma actuator, embedded in a bluff-body burner, on flow downstream of the bluff-body and on flame stabilization of a non-premixed jet flame. The dielectric-barrier discharge (DBD) actuator is operated with AC sine wave and generates a vortex ring downstream of the bluff-body surface. Results show that the presence of the vortex ring alters the local flow velocity and leads to intermittent flame reattachment. Flame reattachment frequency and flame attachment time suggest that the degree of interaction between the flame and the vortex ring has strong dependence on the imposed flow momentum. The dynamic response of flame to the induced vortex ring is represented by a flame describing function (FDF). Given the constant vorticity of the vortex ring, a greater degree of interaction between the vortex ring and the fuel jet leads to more repetitive flame reattachment. Unlike the actuator which induces a vortex ring, the electric field imposes a body force on charged particles in flames and results in a recirculation flow similar to that produced with a bluff-body, but larger and faster. Flames are observed to stably reattach to the bluff-body under the influence of electric field.

Paper ID: 96

Combustion enhancers for ammonia fuelled compression ignition engine

Gabriel J Gotama (The University of Melbourne), Yi Yang (The University of Melbourne), Xingcai Lu (Shanghai Jiao Tong University)

Ammonia fuelled internal combustion engines are a promising technology for decarbonising shipping and heavy-duty road transport. For application in compression ignition engines, a combustion enhancer is

generally required to cope with ammonia's low autoignition reactivity. In this study, the autoignition promoting effect of four ammonia enhancers, diesel, dimethyl ether (DME), hydrogen, and methane, are numerically investigated with ignition delay iso-contours on the temperature-pressure plane. Autoignition timing in homogeneous charge compression ignition (HCCI) engine combustion is further compared for ammonia blended with these enhancers at constant mole fractions and constant energy fractions. At constant mole fraction, diesel is most effective in promoting autoignition, DME is more effective than hydrogen at higher pressures, and both hydrocarbons exhibit negative temperature coefficient behaviour. At constant energy fraction, hydrogen becomes more promoting with the negative pressure dependence, which produces the earliest autoignition timing in the HCCI engine simulation. Methane is the least promoting fuel in all cases. These results suggest that despite being less reactive than diesel and DME as a neat fuel, hydrogen could be a more practical enhancer for ammonia combustion in compression ignition engines.

Paper ID: 97

Semi-empirical models of density jump position and temperature attenuation of smoke layer in horseshoe tunnel fire

Aoi Tanno (Yokohama National University), Yasushi Oka (Yokohama National University)

The present study focuses on the flow properties of the smoke layer in the tranquil flow region in a horseshoe-shaped tunnel under natural ventilation. Small-scale fire experiments have been conducted using a horseshoe-shaped tunnel with 0.275 m in height, 0.41 m in width at floor level and 10 m in length. New semi-empirical prediction formulae to estimate the density jump position and the temperature rise at the position have been proposed by the combination of approximate analytical solutions of a simplified theoretical model and scaled model experiments. The effects of the cross-sectional area and the heat release rate are taken into consideration in these formulae. In addition, a simple correlation for the smoke layer temperature has been proposed in the form of the weighted average of exponential functions. For validation, this correlation has been compared with measurement results obtained from horseshoe-tunnel experiments with different cross-sectional geometries. As a result, it has been confirmed that these new formulae can be applicable to the prediction of the flow properties of the smoke layer originating from a fire source whose average flame height is in the range from about half of the tunnel height to the tunnel ceiling.

Paper ID: 98

The effect of the addition of ammonia on the oxidation of dimethyl ether: an experimental and modeling study

Wang Qiao (Tsinghua University), Liao Wanxiong (Tsinghua University), Haodong Chen (Tsinghua University), Bin Yang (Tsinghua University)

The effects of ammonia (NH_3) addition on the oxidation of dimethyl ether (DME) were investigated experimentally and numerically in a jet-stirred reactor (JSR) at atmospheric pressure in a temperature range of 500–1100 K. The experiments were performed under oxidizing condition (ϕ =0.25) for neat DME and a DME/NH_3 mixture with 10 mol% ammonia blended. Numerous intermediate species were detected and quantified. The results showed that, under the low-temperature oxidation regime (about 500-700 K), the consumption of NH_3 was slow and consequently had little impact on the oxidation behavior of DME. Kinetic

analysis revealed that the consumption of NH_3 in this regime was limited by the dominant pathway of $NH_2+HO_2=NH_3+O_2$. For the intermediate-temperature oxidation regime (about 700-1100 K), the onset temperature for reactions of NH_3 was around 875 K under the studied conditions and the profiles of some hydrocarbon intermediates from the oxidation of DME were significantly affected by the presence of NH_3. The kinetic interaction between DME and NH_3 was related closely to the chemical loop between NO and NO_2, and the consumption of DME was very sensitive to the reaction involved in this loop.

Paper ID: 100

Flame dynamics in a pressurised annular combustor with simultaneous longitudinal-azimuthal thermoacoustic modes

Byeonguk Ahn (NTNU), Håkon Nygård (NTNU), Larry Li (HKUST), Nicholas A Worth (NTNU)

Self-excited longitudinal and azimuthal combustion instabilities are investigated in a pressurised annular combustion chamber with bluff body stabilised methane/hydrogen flames. Stability analysis was performed on a wide range of operating conditions, with unstable longitudinal and azimuthal instabilities found at low and high-power conditions respectively, for a specific hydrogen power fraction. The current study focuses on one specific operating condition, where high amplitude azimuthal instabilities were excited. Both the dynamic onset of instability during an equivalence ratio ramp, and the instability under fixed operating conditions were analysed. Following equivalence ratio ramping both longitudinal and azimuthal modes are excited, and evidence of non-linear mode interaction is observed. Flame dynamics are examined both for simultaneous longitudinal-azimuthal modes, and for predominantly azimuthal modes. When azimuthal modes dominate, strong axial and flapping motions are observed close to the pressure anti-node and node respectively. However, during mixed modes, the flame dynamics significantly differ from those at predominantly longitudinal modes only at the pressure node of the azimuthal mode, due to the superposition of azimuthal and axial velocity oscillations.

Paper ID: 101

Evaluation of the effects of ammonia co-firing of supercritical pulverized coal boilers on plant efficiency and greenhouse gas reduction with economic analysis

Minseob Lim (Korea Institute of Industrial Technology), Jaewook Lee (Korea Institute of Industrial Technology), Won Yang (Korea Institute of Industrial Technology), Jiseon Park (KITECH), Ohchae Kwon (Sungkyunkwan University), Sehyun Baek (Korea Electric Power Research Institute), Junhwa Chi (Korea Electric Power Research Institute), Kyoungil Park (Korea Electric Power Research Institute), Seongil Kim (Korea Institute of Industrial Technology)

In the power generation industry, the application of co-firing the carbon-free fuel ammonia into coal-fired power plant is emerging as a promising method of CO_2 emission reduction. When ammonia co-firing is applied, it is necessary to identify the optimal operating conditions by analyzing the performance of the boiler that changes according to ammonia co-firing. In this study, simulations of an 870 MW_e coal-fired power plant were performed in ammonia co-firing conditions, and the impacts of ammonia co-firing on the greenhouse gas emission and thermal performance of supercritical pulverized coal boiler were analyzed. The process simulation was conducted using two co-firing scenarios (identical excess air ratio and identical adiabatic flame

temperature), both assuming different co-firing ratios of 5, 10, 20, and 30% on heating value basis. The results show that CO_2 emission reduction was increased and plant efficiency was decreased for every increase in the ammonia co-firing ratio. Therefore, there is a trade-off relationship between CO_2 emission reduction and plant efficiency, and in consideration of this, optimal operating conditions were established through economic analysis.

Paper ID: 102

Uncertainty analysis of soot formation in a burner stabilized stagnation flame

Xingyu Su (Tsinghua University), Matthew Cleary (University of Sydney), Hua Zhou (Tsinghua University), Zhuyin Ren (Tsinghua University), Assaad Masri (University of Sydney)

The uncertainty in soot kinetics parameters will lead to uncertainty in the prediction of soot characteristics, including particle size distribution (PSD) and soot volume fraction (SVF). Uncertainty quantification is an important way to evaluate the model performance not only in terms of nominal accuracy but also in terms of confidence intervals. In this work, an uncertainty analysis approach combined with sensitivity analysis and the active subspace method is proposed and demonstrated with a sectional soot kinetics scheme. A laminar benchmark flame, the burner stabilized stagnation (BSS) flame with ethylene as fuel is employed. With the given kinetics uncertainty factor UF=3, the uncertainties of soot volume fractions in the BSS flame are around $SVFmax/SVFmin \approx 3$ at different heights. Furthermore, the importance of each reaction at different soot formation stages is quantitatively revealed and compared along different heights. As expected, at the early stage of soot formation, SVFs are controlled by the nucleation reactions, especially for Rx3 (Ai + Ai = BINi), and surface reactions gradually become important during soot formation. The potential influence of the probe shift on the uncertainty results is also demonstrated. These quantitative uncertainty results are performed for the first time and help reveal the controlling reactions for soot formation.

Paper ID: 103

Tube size effects on diffusion flame extinction in O_2+CO_2 coflow at elevated pressure

Hun Young Kim (KAIST), Nam Il Kim (KAIST)

The combustion characteristics of diffusion flames near the extinction limit under CO_2 diluted oxy-combustion and pressurized condition were investigated experimentally and numerically. The smaller tube and the higher oxygen concentration in a coflowing oxidant made the flame exist at the lower fuel flow rate. In the case of a larger tube in oxy-combustion, the flame was quenched at inside of the tube due to the reduced reaction zone. The dead space between the flame and the tube was related to the minimum fuel flow rate. Flame structures and thermal interaction between the flame and the tube indicate that the flame stabilization can be deteriorated if the flame is located in the tube. With the pressure increase, the flame initially formed above the tube at atmospheric pressure could be quenched in the tube. There was a minimum fuel velocity for the existence of the flame. The flame inside the tube could be changed to a structure closer to a partially premixed flame rather than a diffusion flame.

Paper ID: 104

A study of characteristics of NH_3/n-heptane dual fuel using optical diagnostic

Haifeng Liu (Tianjin University), Tengda Song (Tianjin University), Mingfa Yao (Tianjin University)

As potential alternative fuel, ammonia has been research hotspots in recent years due to its carbon-free molecular structure. The dual fuel combustion of high reactivity fuel and ammonia is a potential solution to solve the drawbacks of ammonia, such as high ignition energy. However, the studies on the characteristics of combustion and emission and relevant mechanisms for dual fuel combustion of ammonia and high reactivity fuel were still limited. In present work, the ammonia/n-heptane dual fuel combustion was studied on a light-duty engine using optical diagnostic techniques. The experiment results indicate that the maximum in-cylinder pressure and the peak of HRR appear in DI-20 case. The earlier DI timing case brings about the lower peak of in-cylinder pressure and HRR due to the over mixing. It is observed that the initial kernels appear near the combustion chamber wall, with orange chemiluminescence. With the delay of DI timing, the flame development mode of the ammonia/n-heptane dual fuel approach changes marginally, but the flame development speed increases. It is also seen that the changes of DI timing affect the flame development marginally. The auto-ignition sites in the initial stage of combustion increase with the increase of DI energy proportion.

Paper ID: 105

Stabilization mechanism for non-premixed lifted flames in a methane-hydrogen blended jet through the laminar to turbulent transition

Dong Seok Jeon (KAIST), Nam Il Kim (KAIST)

The turbulent lifted flame is widely used for the clean combustion system. However, its physical mechanism has yet to be clarified. In this study, the characteristics of lifted flame were estimated. The hydrogen, methane, and their mixture were used as the fuel jet. When the Reynolds number (Re_d) was small (in the laminar regime), a lifted flame could be stabilized below the laminar mixing core and the lift-off height (H_{lift}) monotonically increased with the Re_d. When the Re_d is approximately 2700, a sudden decrease of H_{lift} was observed when the hydrogen concentration ratio (RH_2) is within a suitable range. After that, the H_{lift} increased linearly to the Re_d up to the blowout. When RH_2 became much larger, a new phenomenon was found. H_{lift} decreased drastically and the flame was stabilized at the vicinity of the tube exit. It was even smaller than the turbulent mixing core. When the Re_d increased further, the H_{lift} suddenly jumped at a certain Re_d and increased linearly similarly to the previous turbulent lifted flame theories. Consequently, the stabilization map for the lifted flame was suggested using the laminar, turbulent mixing core, and Re_d.

Paper ID: 106

Accuracy improvements in soot three-parameters fields simultaneous predictions of laminar sooting flames from soot radiation measurements - a multi-task learning approach

Qianlong Wang (Tianjin University), Ting Li (Sun Yat-Sen University), Mingxue Gong (Tianjin University), Haifeng Liu (Tianjin University), MIngfa Yao (Tianjin University)

A novel Trident-Net (T-Net) architecture is designed and assisted for retrieval of high-fidelity soot temperature, volume fraction (SVF) and diameter fields simultaneously from soot radiation measurements in laminar

sooting flames. Uniquely, the T-net is subtly fabricated in one branch of the encoder and three branches of decoders, which enables three adjustable cost functions and the corresponding decoder branch for soot three respective parameter fields. Contrasted with previous Back propagation (BP) and U-net models, the T-Net is more flexible and achieves a higher entire score in terms of individual decoder manipulation. In addition, owing to the generalization performance improvement of multi-task learning, T-Net model demonstrates decent prediction performance under extremely limited train batch size.

Paper ID: 107

Stabilized laminar lifted flame of pure ethane in a non-premixed jet

Gyu Jin Hwang (KAIST), Nam Il Kim (KAIST)

Laminar lifted flames of various fuels have been extensively studied to clarify the flame stabilization mechanism. However, even though ethane satisfies the stabilization criterion of Schmidt number (Sc>1), a stable lifted flame could not be observed experimentally. In our recent studies, an explicit method has been developed to estimate the effective Schmidt number directly from the experimental results of the lift-off height and the fuel jet velocity. Through this, the stabilization mechanism and the stabilization conditions could be clarified, i.e., a triangular stabilization regime (TSR). In this study, the possibility of stable lifted ethane flame was investigated based on the previous stabilization mechanism. Conclusively, a stabilized lifted flame of ethane could be obtained, and the applicability of the flame stabilization theory was confirmed. Lift-off height against the fuel jet velocity was investigated, and the effective Schmidt number was directly estimated from the experimental results.

Paper ID: 108

Bilger's zero release combustion technology as energy storage

Alex Klimenko (The University of Queensland)

This work briefly reviews the energy storage problem that is necessarily associated with the renewable production of energy. The long-term storage, which can suppress seasonal variations in the production and consumption of energy, is connected to the "hydrogen network" that flexibly involves the production, storage transport and consumption of hydrogen and its derivatives (most importantly methane and ammonia). Here, we suggest using Bilger's oxyfuel process for the effective storage of renewable energy in the emerging carbon-constrained environment.

Paper ID: 109

Head-on quenching of an n-heptane/air premixed flame in a stagnation flow

Hibiki Sakuma (Keio University), Takuya Tomidokoro (Keio University), Takeshi Yokomori (Keio University), Hong G. Im (KAUST)

Understanding flame-wall interactions is important for the development of practical combustors. While there are many studies on head-on quenching (HOQ) in a mixture that is initially at rest, there are few studies in a stagnation flow, which is more relevant to the flow field in practical situations. In this study, the HOQ of an n-heptane/air premixed flame in a stagnation flow is numerically investigated for different nozzle velocities and wall temperatures. For both wall temperatures of 300 K and 600 K, the trend of quenching distance with

increasing nozzle velocity changes from increasing to decreasing. This change in the trend is due to the competition of an increasing effect of the flame stretch and a decreasing effect of the convection. Meanwhile, the nozzle velocity at the turning point is higher when the wall temperature is 600 K. This is because, at 600 K, the flame can propagate closer to the wall by itself, therefore the decreasing effect is weakened. These trends of the quenching distance correspond to those of the maximum wall heat flux. Furthermore, around the instant of quenching, the amount of hydrocarbons becomes larger than that in a propagating flame.

Paper ID: 110

Effects of hydrogen addition to CH_4/C_3H_8 on premixed flame propagation in a narrow-gap disk burner

Nam Il Kim (KAIST), Sang Min Lee (KAIST)

Propagation of H_2/CH_4/air and H_2/C_3H_8/air premixed flame was investigated in a Narrow-Gap Disk Burner of which initial volume can be varied. Laminar burning velocities ($SL0$) and Lewis numbers (Le) at the experimental conditions were calculated using GRI-MECH 3.0. $SL0$ increases as H_2 ratio increases, but Le varies differently depending on the equivalence ratio. As the H_2 ratio increases, Le becomes smaller (larger than unity at a lean (rich condition. Therefore, Le of H_2/C_3H_8 premixed flame changes across the unity as the H_2 ratio increases. Next, quenching distances were measured. The quenching distance decreased monotonically as the H_2 ratio increased for H_2/CH_4 premixed flames. However, a trend of variations in the quenching distance of H_2/C_3H_8 premixed flames varied differently, and it was explained based on Le. Flame propagation characteristics changed significantly as the H_2 ratio increased only for lean H_2/CH_4 premixed flame, while there was no notable variation in the other conditions. Especially in the cases of H_2/C_3H_8 premixed flames, it was expected that the flame oscillation at the lean (rich condition would become stronger (weaker as the H_2 ratio increases, because Le changes across the unity. However, such variations could not be observed.

Paper ID: 111

Modelling of a turbulent premixed flame series using an MMC-LES model with a shadow position reference variable with locally adjusted model parameters

Yashar Shoraka (The University of Sydney), Sebastian Galindo Lopez (The University of Sydney), Matthew Cleary (The University of Sydney), Assaad Masri (The University of Sydney), Alex Klimenko (The University of Queensland)

This article introduces a new Multiple Mapping Conditioning (MMC) probability density function model for Large Eddy Simulation (LES) of turbulent premixed flames. By imposing locality in a shadow-position space, the model inhibits non-physical mixing over the flame front. An effective diffusion coefficient is introduced in the shadow position proportional to the ratio of the reference turbulent flame speed to the laminar flame speed estimated by the model parameter λ. Previously, a global and constant value for λ was used in simulations, and results showed substantial sensitivity to its variations. Therefore, λ is evaluated locally using a wrinkling factor model here. The performance is assessed against the experimental data reported for a laboratory-studied piloted premixed flames series. Three methods are assessed for calculating the sub-filter mixing time scale to improve the prediction of actual turbulent propagation speed by accounting for the

interaction between mixing and combustion. Results demonstrate that λ can control turbulent propagation speed without changing flame topology. Furthermore, it is shown that the local evaluation of λ in conjunction with an appropriate method for evaluating the sub-filter scale mixing time can accurately predict the mean flame length.

Paper ID: 112

Bubble nucleation and bursting in the heated molten polymers

En Nagatsu (Toyohashi University of Technology), Takuya Yamazaki (Toyohashi University of Technology), Tsuneyoshi Matsuoka (Toyohashi University of Technology), Yuji Nakamura (Toyohashi University of Technology)

The "internal" gasification process of heated thermoplastic material occurring inside molten matter is presented as bubble nucleation. In this study, a test system for identifying the nucleation formation process is developed wherein a 1.5 mm thick polymer slab is used as the test specimen and a ceramic heater is used as the heat source to initiate bubble nucleation. The heating conditions (surface temperature) are varied in order to control the nucleation appearance. Together with the heat transfer model and 3-points temperature measurements with fine thermocouples, the nucleation thermal condition is discussed. It is found that nucleation randomly appears yet does so nearly several millimeters below the heating surface. With the gas-molten interface gasification, the bubble grows in time and its shape elongated upward, eventually reaching the top surface to abruptly release the gas (bursting). The nucleation temperature is found not to be constant, rather, weakly increased with the adopted heating temperature. It is suspected that there is the lowest nucleation temperature based on the measured result. However, there is still room to discuss this in detail.

Paper ID: 113

Characteristics of laser-induced breakdown plasma as a combustion diagnostic tool and an ignition source under various density conditions

Jieun Kang (Korea University), Seongkyun Im (Korea University)

The plasma characteristics of laser-induced breakdown (LIB) were experimentally studied under various pressure conditions for applications such as a combustion diagnostic tool and an ignition source. For the quantitative comparative study of single-pulsed laser-induced breakdown (SPLIB) and dual-pulsed laser-induced breakdown (DPLIB), N II spectra and direct imaging of sparks from an intensified camera were analyzed. Electron temperature and number density were obtained by applying a nonlinear least-squares method to fit the calculated spectrum to the measured spectrum. The spectrum peak intensity of DPLIB tends to be increased than that of SPLIB, but SNR is only improved at around ambient pressure 120 ns after the breakdown. Due to higher energy accumulation and the higher collision frequency, plasma size increased as the pressure increased above 1 bar. With sufficient laser energy, DPLIB can have faster thermal diffusion than SPLIB because of a larger plasma size. For low-pressure conditions, the plasma temperature of DPLIB is higher than that of SPLIB, but for high-pressure conditions, DPLIB has a lower peak temperature than SPLIB, which is advantageous as an ignition source due to low radiative heat loss. For all pressure conditions, DPLIB has a higher electron density than SPLIB.

Paper ID: 114

Effects of the coaxial air on flame stabilization of methane/hydrogen non-premixed flames under elevated pressures

Jiseop Lee (KAIST), Nam Il Kim (KAIST)

To achieve zero CO_2 emission, hydrogen addition to methane flame under high pressures will become a practical technology that can be directly applied to the current combustion systems such as gas turbine. One of the representative issues is soot emission under high pressures, and a practical method is using a lifted flame. In this study, characteristics and stabilization conditions of turbulent lifted flames of hydrogen and methane mixture were experimentally investigated using coaxial tubes in a surrounding tube under elevated pressures. Flame stabilization characteristics were divided into three modes; inner attached, outer attached, and inner lifted flames. Especially the stabilization mechanism of the inner lifted flame was investigated in more detail because it could reduce the soot emission and was stable even at relatively high flow rates. The upper boundary of the inner lifted flame (or blow-off limit) was related to the turbulent intensity. In addition, the lower boundary of the inner lifted flame was related to the flammability limits of a premixed flame. With these two criteria, the inner lifted regime could be predictable even at higher pressure or hydrogen ratio.

Paper ID: 115

A tungsten oxide thin film carbon monoxide gas sensor by RF sputtering

Hao Yuan Cheng (National Kaohsiung University of Science and Technology), Ting-Jen Hsueh (National Kaohsiung University of Science and Technology)

Carbon monoxide (CO) is the most lethal factor in fires. Carbon monoxide is invisible, colorless, and odorless. It often becomes the biggest invisible killer in the fire scene. The risk of accidents is reduced through the WO3 gas sensor, which is detected by the characteristics of reducing gases Gas, changing the operating temperature of the material to affect the response size.

Paper ID: 116

Experimental and numerical study on stratified combustion with hydrogen enrichment

Ruihan Ge (Xi'an Jiaotong University), Erjiang Hu (Xi'an Jiaotong University), Xin Lv (Xi'an Jiaotong University), Chenglong Tang (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University)

A study on ethanol stratified lean combustion with H_2 enrichment in constant volume vessel under different ambient pressures and temperatures is conducted. The combustion and spray characteristics in experiment and spray numerical simulation are obtained to investigate the stratified combustion. The experiment shows that overall combustion pressure is higher under lower temperature conditions and increases with elevated pressure, the rapid burning durations which stands for stratification degree are similar under different pressures and first increase then decrease with ambient temperature. The simulation further investigated the factors (evaporation, fuel density distribution and turbulent kinetic energy) effected the stratified combustion. The results indicate that the spray morphology around the ignition position has significant influence on it. While the spray characteristics change slightly under different pressures, the corresponding rapid burning durations are similar. While the ethanol evaporated more sufficiently, the unburned liquid/gas mixture is closer to homogenous status and suppressed the advantage of stratified combustion. When the ambient temperature and fuel density

around ignition position are well balanced, stable combustion under lean-burn condition can be achieved.

Paper ID: 117

Experimental and kinetic studies of N_2O in elevated pressure ammonia oxidation

Haochen Zhan (Xi'an Jiaotong University), Shuming Li (Xi'an Jiaotong University), Geyuan Yin (Xi'an Jiaotong University), Erjiang Hu (Xi'an Jiaotong University), Zuohua Huan (Xi'an Jiaotong University)

In this research, ammonia oxidation experiments were carried out on the flow reactor close at the operating pressure of the engine works, focusing on the production and consumption of N_2O. The pressure was 5.0 MPa, the temperature from 600-1250 K and the equivalence from 0.13-1.0. Simulations and kinetic analyses were carried out using kinetic models of ammonia oxidation published in recent years, evaluating the predictive ability of models for different products at elevated pressure conditions. The branching ratios for the reactions of NH_2 and NO_2 were modified according to the calculations by recent research. Optimized model with the addition of the missing reaction paths captured the experimental data well at different equivalence ratios.

Paper ID: 118

Numerical simulation of a non-reacting air-blast ethanol spray using explicit volume diffusion method

Jiayue Yu (The University of Sydney), Sebastian Galindo-Lopez (The University of Sydney), Matthew Cleary (The University of Sydney), Agisilaos Kourmatzis (The University of Sydney), Bosen Wang (Beihang University, China)

In multiphase turbulent flows, the smallest diffusion scale does not exist and approaches zero. The traditional volume of fluid method therefore usually suffers from significant grid sensitivity issues when the grid resolution is refined. This is because of changes in the resolved interfacial dynamics. The explicit volume diffusion (EVD) concept involves a volume averaging process of the governing equations over an explicitly defined physical length scale associated with an interfacial characteristic length. Physical diffusion is added into the system to thicken the interface and account for sub-volume fluctuations due to both turbulence and interfacial dynamics. By not varying the explicit volume length scale while refining the numerical grid, the explicit volume diffusion overwhelms the numerical diffusion and numerical convergence can be assured. EVD has been validated against low Weber number laminar and turbulent jets. Here, a higher Weber number (We = 77) non-reacting ethanol spray case from a standard coaxial air-blast atomiser (Sydney University Needle Burner, SYNSBURN) is conducted using the EVD method to evaluate its capacity to capture the dynamics of two-phase flows in the atomisation regime. The temporally averaged volume fraction and root mean square of the fluctuations are examined and a good agreement with the experimental observation is achieved with minor differences.

Paper ID: 119

Study of ion current characteristics in premixed ammonia-air flames

Dhaminda N Hewavitarane (University of Kitakyushu), Sadami Yoshiyama (University of Kitakyushu), Jotaro Arishima (University of Kitakyushu), Mitsuhiro Izumi (Diamond & Zebra Electric Mfg. Co. Ltd), Tustomu Kusuhara (Diamond & Zebra Electric Mfg. Co. Ltd), Shigeki Hasegawa (Diamond & Zebra Electric Mfg. Co. Ltd)

This study deals with the non-carbon fuel Ammonia (NH3) and the characteristics of the ion current in its air premixed flames. A novel method for measuring the ion current is proposed in such a stagnated flat flame. a clear relationship is seen to exist between the ion current, the equivalence ratio and NO in the burned gasses of Ammonia-Air pre-mixed flames. Experimental results show that as the equivalence ratio increases from 0.89 to 1.19, the peak value of ion current decreases. In order to clarify the reason for this trend, elementary reaction calculations using a newly developed ionic reaction mechanism were performed. The ion concentration trends of the ion species NO+, H3O+, O+ and N+ are seen to be similar to the ion current trend in the rich zone with NO+ being the dominant ion species. However, results of numerical calculations give the ion concentration peaks at $\varphi \approx 1.01$ whereas the experimentally measured ion current peak is at $\varphi \approx 0.95$.

Paper ID: 120

Effect of H_2 addition on laminar burning velocity of NH_3/DME blends by experiments and a reduced mechanism

Li Huizhen (University of Science and Technology of China), Huahua Xiao (University of Science and Technology of China)

Blending dimethyl ether (DME) into ammonia (NH_3) can efficiently enhance the combustion of pure NH_3, and has attracted increasing attention. Partial dissociation of NH_3 can convert NH_3/DME mixtures to NH_3/DME/H_2 mixtures. This work measured the laminar burning velocity of NH_3/DME/air mixtures for two blend ratios (80/20 and 60/40) with various H_2 additions (0%, 20%, and 40%) at phi = 0.7~1.7, 0.1 MPa, and 298 K using a spherical constant-volume combustion method. A kinetics mechanism was reduced according to our published detailed mechanism. The results show that the existence of H_2 can significantly increase the laminar burning velocity of NH_3/DME/air mixtures. Relative increase (E_{SL}) in laminar burning velocity presents non-monotonic tendency with increasing equivalence ratio for various H_2 addition, and the peak value of E_{SL} appears at phi = 1.5. This can be attributed to the dominant effect of C-contain and N-contain reactions on E_{SL} rather than H-O reactions at rich burn side.

Paper ID: 122

Unsteady extinction of ammonia premixed flames against an isothermal wall

Takuya Tomidokoro (Keio University), Takeshi Yokomori (Keio University), Hong G. Im (KAUST)

This study numerically investigates an unsteady extinction of a premixed stagnation flame convected toward an isothermal, non-reacting wall under increasing flow velocity. Ammonia is used as a fuel for future studies on the emission characteristics during the quenching process. The results reveal that the moment of extinction is well characterized by the local Peclet number Pe_L≈3, which is analogous to the well-known head-on quenching criterion. Meanwhile, when the rate of increase in the flow velocity becomes high, the local Karlovitz number Ka_L at the moment of extinction can be as large as O(10), which is much larger than the steady extinction criterion of Ka_L≈1. This is caused by the delayed response of the flame movement. With increasing Ka_L, the influence of flame stretch on the extinction process is amplified. A regime diagram based on the local flame thickness and consumption speed is proposed. It is found that the unsteady extinction mechanism transitions from an enthalpy-loss-driven mode to a residence-time-driven mode with increasing Ka_L, and the transition behavior depends on the effective Lewis number of the mixture.

Paper ID: 123

Flame spread over thin hollow cylindrical fuels and its comparison with thin planar fuels

Vipin Kumar (Indian Institute of Technology Madras), Amit Kumar (IIT Madras), Manu B V (Indian Institute of Technology Madras), Yusuke Konno (Hokkaido University), Osamu Fujita (Hokkaido University)

Downward flame spread over thin cellulosic fuel is investigated in normal gravity and microgravity environments to understand the effect of fuel shape and opposed convective flow on flame spread rate. Hollow cylindrical fuel with diameters of 19 mm and 38 mm and corresponding planar fuels of width of 20 mm and 40 mm, are selected for investigation under different effective opposed flow conditions. The experiments are conducted under atmospheric condition of oxygen concentration and pressure. All the microgravity test were conducted using the 2.5 s drop tower available at the National Centre for Combustion Research and Development (NCCRD), IIT Madras, India. It is observed that flame spread rates are higher than for the hollow cylindrical fuels compare to the corresponding planar fuel widths. Further, as the diameter of the fuel increases, the flame spread rate increases. The effect buoyant flow on flame spread rate are also discussed.

Paper ID: 124

Numerical analysis of hydrogen peroxide addition and oxygen-enhancement for methane combustion

Annas Fauzy (National Cheng Kung University), Guan-Bang Chen (National Cheng Kung University), Fang-Hsien Wu (National Cheng Kung University), Tai-Hui Lin (National Cheng Kung University)

Methane (CH_4)/air lean combustion can be enhanced by increasing an oxidizer concentration, like oxygen (O_2)-enriched, or adding a strong oxidant to the reactant. Hydrogen peroxide (H_2O_2) is a strong oxidizer that yields O_2, steam, and appreciable heat after decomposition. This study numerally investigated and compared the effects of adding H_2O_2 and O_2-enriched conditions on the adiabatic flame temperature, laminar burning velocity, flame thickness, and heat release rates of CH_4/air combustion using the San Diego Mechanism. The result showed that in the fuel-lean conditions, the adiabatic flame temperature changed upon H_2O_2 addition > O_2-enriched scenario to O_2-enriched scenario > H_2O_2 addition with increasing α. This transition temperature was not affected by the equivalence ratio. Adding H_2O_2 enhanced the laminar burning velocity of the CH_4/air lean combustion more than the O_2-enriched scenario. Further, the laminar burning velocity had a quasi-linear correlation with (OH)max in the flame. The maximum heat release rate was in the lower temperature for H_2O_2 addition and the higher temperature for the O_2-enriched scenario. The flame thickness was significantly reduced upon adding the H_2O_2. Finally, the dominant reaction to the heat release rate changed from the reaction of $CH_3 + O \leftrightarrow CH_2O + H$ in the CH_4/air or O_2-enriched scenario to the reaction of $H_2O_2 + OH \leftrightarrow H_2O + HO_2$ in the H_2O_2 addition scenario.

Paper ID: 125

Non-thermal plasma catalytic NH_3 dehydrogenation over ceria-based catalysts

Yibo Gao (Xi'an Jiaotong University), Erjiang Hu (Xi'an Jiaotong University), Geyuan Yin (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University)

Plasma-catalytic NH_3 dehydrogenation (ND) to generate zero-carbon hydrogen (H_2) over low-cost catalysts has been a hotspot area. In this work, ceria-based catalysts were prepared by a facile deposition-precipitation

method. Bimetal (FeCo, FeNi and CoNi) doping CeO_2-based catalysts exhibit better catalytic activity than that of single-metal (Fe, Co and Ni) doping catalysts. Based on the strong metal support interaction (SMSI), more electrons are transferred from support to active metal sites. And the addition of non-thermal plasma (NTP) further enhances reaction rate of ND. In the catalyst and plasma, $FeCo/CeO_2$ catalyst showed the highest NH_3 conversion in the prepared catalysts, which achieves 100% conversion at 550 °C. This work directly demonstrates the synergistic promotion effect between non-thermal plasma and ceria-based catalysts over NH_3 decomposition.

Paper ID: 126

Kinetic study on ammonia oxidation at fuel-rich conditions with H_2O addition using a micro flow reactor with a controlled temperature profile

Kenta Tamaoki (Tohoku University), Yuki Murakami (Tohoku University), Keisuke Kanayama (Tohoku University), Takuya Tezuka (Tohoku University), Hisashi Nakamura (Tohoku University)

The effects of H_2O on NH_3 oxidation and H_2 production for $NH_3/O_2/H_2O/Ar$ mixtures at stoichiometric and fuel-rich conditions are investigated using a micro flow reactor with a controlled temperature profile (MFR). Species measurements of NH_3 and H_2 are conducted with a quadrupole mass spectrometer and a gas chromatograph, respectively. Two cases of H_2O fraction in diluents (0% or 20%) are tested and compared at well-defined temperature profiles (1100–1400 K in maximum). Measured NH_3 and H_2 profiles are independent of H_2O concentration. Chemical kinetic model is developed based on literature, which predicts experimental results quantitatively. According to reaction path analyses, H radical is major source of H_2 and R1: $NH_3 + H = NH_2 + H_2$ is dominant for H_2 production. H_2 production is controlled by the competition for H radical between R1 and R2: $H + O_2 = O + OH$. When equivalence ratio increases, R2 is inhibited because of decrease in O_2 and then H_2 production by R1 increases. Furthermore, H radical consumption by $H + O_2 (+M) = HO_2 (+M)$ is minor. As a results, the prediction shows little effects of H_2O on NH_3 oxidation and H_2 production although H_2O has the large third-body collision efficiency.

Paper ID: 127

Effect of louvre hole size on the combustor efficiency

Liang-Chun Liu (NCSIST), Chi Chien Wu (NCSIST), Yu-En Wu (NSCIST), Chun-Hua Kuo (NSCIST)

The impact of louvre hole size to the combustion efficiency of a annular combustor is investigated with experimental verification and numerical simulation. Two sets of liner, each with different louvre hole sizes, are manufactured and tested for combustion experiments. A simplified 1/6 combustor is simulated with CFD, while numerical and experimental results both show that the smaller louvre hole size range causes an increase in combustion efficiency of 2~3%.

Paper ID: 128

Numerical prediction of the central recirculation zone in a v-shaped swirling flame

Qiuxiao Wang (Shanghai Jiao Tong University), Yongzhi Ren (Shanghai Jiao Tong University), Xi Xia (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University)

This study employs Large-eddy simulation (LES) and the Flamelet Generated Manifold (FGM) combustion

model to numerically predict the emergence of the central recirculation zone (CRZ) in a V-shaped premixed swirling flame. The computed swirling flow and flame features agree well with our previous measurements, verifying that the present numerical simulation is properly performed to capture the complex swirling flow and flame behaviors. The flame temperature is then extracted from the numerical results for estimating the heat transfer coefficient of V-shaped swirling flames. Based on a proposed simplified heat loss model, the temperature and viscosity of the inner shear layer (ISL) surrounding the CRZ can be estimated. This further enables the calculation of a relationship between the ISL circulation Γ and viscosity ν_s , where a linear boundary exists between the cases with and without CRZ. The result points to a common critical Re_s , determined to be around 609 based on the boundary line's slope, which serves as a general criterion to predict CRZ emergence.

Paper ID: 129

Equivalence ratio measurement by LIBS in double hydrogen jets at gasoline engine-like conditions

Jungho Justin Kim (KAIST), Seong-Young Lee (MTU), Sang Uk Lee (KAIST), Choongsik Bae (KAIST)

Direct injection technology has been known as the best option for applying highly diffusive hydrogen in combustion engines while limited studies on hydrogen jet behavior have been done to elucidate engine design and injection parameter optimization. In order to overcome the intrinsically weak momentum of the hydrogen jet which leads to jet contraction in the hollow-cone shape injection, the double injection strategy is considered in the currently study. Characteristics of stratified hydrogen direct injection were analyzed in a constant volume combustion chamber. The mixing of the hydrogen and surrounding gas during single and double injection jet schemes was quantitively measured using the calibrated laser-induced breakdown spectroscopy (LIBS) inside the hydrogen hollow-cone jet. Analysis of jet propagation was also done with schlieren photography. It was found that double injection strategy promoted the higher probability of flame ignitability by increasing the jet width by splitting the jet mass.

Paper ID: 131

Prediction of fire-induced ceiling jet characteristics based on artificial intelligence

Yanfu Zeng (The Hong Kong Polytechnic Univerisity), Tianhang Zhang (The Hong Kong Polytechnic Univerisity), Xinyan Huang (The Hong Kong Polytechnic Univerisity)

Ceiling jet behaviour is fundamental of the building fire detection design. Alpert's semi-empirical correlations are widely used to calculate the ceiling jet characteristics, but they are limited to describing steady-burning fires. The numerical fire modelling reveals more details of the transient fire processes, but it is time-consuming and requires high computational costs. This work develops an Artificial Intelligence (AI) model which aims to provide a quick prediction of the gas temperature and velocity in ceiling jet flow under transient fire scenarios. A numerical database is first constructed to collect fire data by considering key attributes. Then, a deep learning model is trained which can predict the evolution of the gas temperature and velocity for T-square growth fires within 10 s, while accuracy is up to 93%. It also demonstrates good prediction performance in the steady burning and decay stages. The AI model allows a quick and accurate prediction of the detector response and can contribute to the improvement of building fire detection design.

Paper ID: 132

Linear burn rate of gelled hydroxylammonium nitrate aqueous solutions

Yu-Jia Chen (National Cheng Kung University), I-You Tsai (National Cheng Kung University), Yan-Ze Song (National Cheng Kung University), Ming-Hsun Wu (National Cheng Kung University)

The burn rate of hydroxylammonium nitrate (HAN) aqueous solution is relatively low when the boiling temperature of the water content is lower than the decomposition temperature of HAN at lower pressures. However, the burn rate abruptly surges after the pressure exceed a threshold value, at which the boiling temperature is higher than the decomposition temperature. As a result, additional fuels and stabilizers have to be added in HAN-based liquid monopropellants to improve the burning characteristics. Fumed silica can absorb water in HAN aqueous solution through the formation of hydrogen bonds between the silica particles and water molecules. In the present effort, hydrophilic fumed silica (CAB-O-SIL M5) was added into 80 wt.% HAN aqueous solution to produce HAN gel. Burn rate behavior of the gelled HAN solution was experimentally studied via strand burner tests at pressures between 0.1-3.1 MPa using a pressure chamber with observation windows. It was found that gelation of HAN aqueous solution using fume silica could effectively eliminate the burn rate jump between 1.1-1.6 MPa typically occurs in the HAN aqueous solution.

Paper ID: 134

Raman/Rayleigh measurements in NH_3/H_2 flames at atmospheric pressure: comparison between 1-component and 2-component approach

Hao Tang (KAUST), Diana Ezendeeva (KAUST), Gaetano Magnotti (KAUST)

This study reports the Raman/Rayleigh technique for measurements of major species and temperature in laminar NH_3/H_2/-air flames at atmospheric pressure by using a 1-component and 2-component approach for interference treatment. The experimental setup and data processing for the two approaches are introduced. Finally, the measurement accuracy and precision of the two approaches in laminar flames are compared and discussed.

Paper ID: 135

Emission characteristics of polycyclic aromatic hydrocarbons from five scale of heavy fuel oil fire

Chi-Fu Yeh (Hwa-Ying Environment Technical Consultants Co., Ltd), Ming-Jen Chen (Fooyin University), Kuang-Chung Tsai (National Kaohsiung University of Science and Technology)

Polycyclic aromatic hydrocarbons (PAHs) are mainly produced through combustion behaviours, which affects the environment and humankind's health. In this study, five burning scales of 0.2, 0.6, 1.1, 1.2, and 1.5 m were simulated to investigate the physical and chemical characteristics of 16 PAHs emissions during heavy oil combustion. The results showed that the total PAHs emission factor (EF) of the coarse particle (>2.28μm) and fine particle (<2.28μm) in five scales of heavy oil combustion ranged from 3.78 to 74.3 mg kg-1 and 71.7 to 220 mg kg-1, respectively. In addition, the highest EF of coarse and fine particles appeared in a 1.1m oil pan. The highest total PAHs emission factor was observed at the flame temperature of 945 °C (1.1 m) and decreased after that. In CO/CO2 factor, the highest total PAHs EF appeared at 1.1m (0.0337) and then decreased. At the flame height, the highest total PAHs EF occurred at the 1.1m scale (1.23m) and then decreased. The total PAHs TEQ of coarse and fine particles ranged from 0.079 to 18.6 BaPeq-TEQ mg kg-1 and 15.2 to 63.2

BaPeq-TEQ mg kg-1, respectively. The above results showed that the characteristics of PAHs emissions are affected by combustion temperature, CO/CO2 and flame height in different combustion scales.

Paper ID: 137

Spray characteristics of hydro-processed renewable diesel on constant volume combustion chamber

Warit Abi Nurazaq (National Cheng Kung University), Wei-Cheng Wang (National Cheng Kung University), Cho-Yu Lee (National Sun Yat-sen University), Manida Tongroon (MTEC,NSTDA)

Hydro-processed renewable diesel fuel has a high potential to replace conventional diesel for combustion engine applications. Therefore, some researchers have investigated that HRD has gained popularity since it performs better than traditional fuels to improve combustion and decrease emissions. In this work, the spray characteristics, including spray penetration and cone angle of HRD, were investigated using a constant volume combustion chamber equipped with high temperature and pressure control tools to provide the condition on combustion engine condition. In addition, the shadowgraph imaging technique was used to capture the spray penetration. The results show that the spray penetration decreases with increasing temperature, and the high temperature improves the vaporization of fuel inside the chamber. High injection pressure tends to improve spray penetration. Moreover, ambient pressure significantly affects how spray penetration develops. Spray length penetration was reduced with increasing ambient pressure. On the contrary, the spray angle was slightly constant when achieving steady-state conditions.

Paper ID: 138

Assessing the performance of multi-component surrogates in replicating combustion characteristics of gasoline fuel.

Inna Gorbatenko (King Abdullah University of Science and Technology), Abdullah S AlRamadan (Aramco), Yohan Chi (Hyundai Motor), Donghee Han (Hyundai Motor), Junseok Chang (Saudi Aramco), S. Mani Sarathy (KAUST)

Gasoline is primary choice for light duty applications globally. However, its compositional complexity makes it difficult to experimentally and computationally study its combustion characteristics. Consequently, surrogate fuels are adopted to represent the behavior of real fuels in experimental and computational investigations. This study assesses an existing octane blending model for ethanol/gasoline surrogates in formulate a surrogate to replicate auto-ignition characteristics and speciation data of real gasoline in a computational framework. The model is capable of accurately capturing the temperature dependent auto-ignition behavior at both lean and stoichiometric conditions. However, predictions of evolution of major products and intermediates in a jet stirred reactor require further improvements.

Paper ID: 139

Effect of a shear flow on the stability of premixed and non-premixed flames

Joel Daou (University of Manchester), P Rajamanickam (University of Manchester), A Kelly (University of Manchester), J Lande (University of Manchester)

The coupling between shear-enhanced diffusion (Taylor dispersion) and flame instabilities is a scientifically rich research topic whose investigation has only been recently initiated. Background and reports on related

investigations can be found in [1, 2] in the context of premixed combustion. The current communication will report recent development in this topic for both premixed and non-premixed flames. The focus of the work is on the effect of Taylor-dispersion on the thermo-diffusive instabilities of premixed and non-premixed flames.

The problem is addressed both analytically and numerically in the framework of a constant density two-dimensional model accounting for shear-enhanced diffusion. The analytical investigation is based on large activation energy asymptotics. A linear stability analysis is carried out leading to a dispersion relation involving two main parameters: the Lewis number Le, and the Peclet number Pe. Stability diagrams are determined in terms of these and other pertinent parameters. Particular attention is devoted to the nature of the bifurcations observed in order to identify various cellular and oscillatory flame patterns. One of the interesting results obtained is the demonstration that Taylor dispersion can significantly alter the critical conditions for the onset of the classical cellular instability expected in mixtures with sub-unity Lewis numbers, leading to its occurrence in Le>1 mixtures if the Peclet number is above a critical value. This novel result seems to provide an explanation of the unexpected appearance of cellular structures called diffusion flame streets in non-premixed micro-combustion devices [3, 4].

Paper ID: 140

Effects of ethylene penetration height and equivalence ratio on combustion instabilities in a scramjet model combustor with a cavity flame holder

Shoya Yasunaga (University of Tokyo), Shota Nishimoto (University of Tokyo), Jeonghoon Lee (University of Tokyo), Shinji Nakaya (The University of Toky), Mitsuhiro Tsue (University of Tokyo)

Effects of the ethylene penetration height and the equivalence ratio on combustion were experimentally investigated using a scramjet model combustor with a cavity flame holder. Combustion behaviors were observed for the injection orifice diameters: d from 2, 3, and 4 mm the equivalence ratio ϕ from 0.15 to 0.23 at a stagnation temperature of 1900K and Mach speed of 2. CH* chemiluminescence and shadowgraph images were observed simultaneously with high-speed video cameras, and the high-resolution images and shock parameters extracted from shadowgraph images (observables) were mapped into low- dimensional latent variables using SGPLVM (Shared Gaussian Process Latent Variable Model). Results indicated that an oscillation between ramjet and scramjet modes was observed for ϕ= 0.17 to 0.20 and d= 3 or 4 mm. However, at d= 2 mm, another oscillation between shear-layer and lifted shear-layer modes was observed with an oscillation frequency which was different from that of ram-scram oscillation. These combustion images were classified in different clusters of the two-dimensional latent space obtained with SGPLVM, suggesting that the mechanisms driving each oscillation are different. In addition, transitions between the clusters were confirmed depending on ϕ , corresponding to the variation of CH* chemiluminescence images and shock parameters.

Paper ID: 141

Autoignition in a premixed jet flame in a crossflow

Harikrishna Tummalapalli (University of New South Wales), Evatt Hawkes (University of New South Wales), Dominic Ma (University of New South Wales)

In this work, we conduct an analysis of flame stabilisation of a premixed jet flame in a vitiated cross flow, a

configuration that closely represents the second stage of an axially staged gas-turbine combustion system. A premixed methane-air jet with an equivalence ratio of 0.7 is injected into a vitiated cross flow comprising combustion products from a methane-air mixture at an equivalence ratio of 0.5 and atmospheric pressure. The direct numerical simulation is performed using a compressible high-order accurate numerical solver (S3D). The simulation results show a lifted flame quasi-statically anchored on the leeward side. At the mean flame base, independent ignition kernels are formed indicating an autoignition stabilised flame. The rationale behind this preferential leeward autoignition is presented. Finally, it is shown that the ignition kernels at the mean flame base transition into premixed flame fronts, which presents significant challenges to the current turbulent combustion models.

Paper ID: 142

Investigation of pressure effects on cool flame ignition temperature through the gas temperature-compensated HCHO-TDLAS measurement

Minhyeok Lee (The University of Tokyo), Gengyu Li (The University of Tokyo), Yuji Suzuki (University of Tokyo)

Effects of pressure on cool flame ignition characteristics were investigated through a tunable diode laser absorption spectroscopy (TDLAS) technique. DME premixed cool flames were formed near the heated wall, of which temperature was ramped up at a constant rate. The ignition process of the cool flame was identified by measuring the HCHO mole fraction under mildly-elevated pressure conditions. The HCHO-TDLAS and two-line H2O-TDLAS for gas temperatures were simultaneously carried out to accurately measure the HCHO mole fraction. The effects of different pressures and equivalence ratios on the cool flame ignition temperature were investigated.

Paper ID: 143

In situ measurement of NO and NH_3 in combustion emissions using mid-infrared laser absorption sensor

Kun Duan (The Chinese University of Hong Kong), Yongbin Ji (The Chinese University of Hong Kong), Zhimin Lu (South China University of Technology), Shunchun Yao (South China University of Technology), Ke Xu (LaSense Technology Limited), Xiang Zhang (Guangdong Provincial Institute of Metrology), Zhiming Huang (Hua Nan Calibration Limited), Wei Ren (The Chinese University of Hong Kong)

We report the in situ detection of high-temperature NH_3 and NO using a mid-infrared laser absorption sensor, which is suitable for combustion emissions monitoring at the SCR (selective catalytic reduction) exhaust. Two quantum cascade lasers (QCL) are combined to probe the intense absorption features at 1103.45 cm-1 and 1929.03 cm-1 for NH_3 and NO detection, respectively. Two beams from QCLs are coupled into a single hollow-core fiber and delivered to an open-path, single-ended optical probe, which can be inserted into hostile environments for in situ gas detection. The gas concentration is determined by calibration-free wavelength modulation spectroscopy (CF-WMS), which is validated by measuring gas mixtures of known concentrations at varied conditions. Allan deviation analysis reveals detection limits of 30 ppb under 100 s average time and 14 ppb under 70 s were achieved for NO and NH_3, respectively. Simultaneous and real-time measurement of NO and NH_3 is demonstrated at the SCR exhaust of a coal-fired power plant.

Paper ID: 144

An experimental and modeling study on the combustion characteristics of nitrates/nitrites in an RCM

Zhaohan Chu (Tsinghua University), Wanxiong Liao (Tsinghua University), Zhongkai Liu (Tsinghua University), Bin Yang (Tsinghua University)

Nitrogen-contained fuels have commanded considerable scientific interest in recent years as a primary source of NO_x in combustion and for their potential use as energetic propellants. Despite experimental works previously conducted for nitrogen-containing compounds combustion, the ignition data of two typical nitrogen-contained fuels, nitrates/nitrites, are still scarce. A comprehensive experimental and kinetic study on the oxidation and decomposition of nitrates and nitrites was performed. Ignition delay times and pressure profiles were measured in a rapid compression machine (RCM) under 5-8 bar at temperatures from 550 to 600 K with varying concentrations of O_2. Three-stage heat release behaviors were observed for both nitrates and nitrites fuels under specific conditions. Auto-ignition phenomenon was observed for the nitrate fuel decomposition process. A detailed kinetic mechanism was constructed, with which the observed combustion characteristics of these two fuels were explained. Incomplete combustion affected the total heat release. Nitrogen-contained intermediates participate in the combustion process resulting in the three-stage heat release in the oxygen-rich condition. Auto-ignition phenomenon is caused by NO_2 acting as an oxidant during the decomposition process, which is unique to nitrates fuels.

Paper ID: 145

Exemplar-based clustering algorithms for experimental datasets based on affinity propagation and global sensitivity analysis

Yiru Wang (Tsinghua University), Zijun Zhou (Tsinghua University), Keli Lin (Tsinghua University), Chenyue Tao (Tsinghua University), Chung K. Law (Princeton University), Bin Yang (Tsinghua University)

The combustion kinetics model's accuracy is crucial for studying the combustion phenomenon and the numerical simulation in practical engineering problems. To reduce the uncertainty of model parameters, one of the key factors affecting the accuracy of prediction, Bayesian methods are usually used to carry out uncertainty constraints based on experimental data. With the rapid growth of experimental data, using all experimental data for optimization is redundant and time-consuming and may lead to data consistency problems. Therefore, this study proposes a new method for clustering experimental datasets and selecting representative experimental conditions based on affinity propagation and global sensitivity analysis. In this method, the global sensitivity coefficient is first obtained through global sensitivity analysis to characterize the reactivity of the kinetic model under different experimental conditions. The similarity coefficient defined based on the global sensitivity is used to characterize the similarity of the sources of model uncertainty under different experimental conditions. Affinity propagation enables the experimental dataset to be automatically clustered into several classes without specifying the number of classes in advance. This method innovatively introduces the consideration of model and experimental uncertainty under different conditions to obtain better optimization results.

Paper ID: 146

Characteristics of fuel vaporization, combustion and flows of air, fuel vapor and liquid during ethanol-pool fire

Kenshin Kobayashi (Yamaguchi University)

To elucidate the mechanism of small-scale pool fires from the perspective of fire safety, this study investigated the characteristics of fuel vaporization and combustion based on the flow-field measurement both in the gas and liquid phases using PIV measurement. The results show that the flame height oscillated at about 8 to 15 Hz. Both the maximum flame height and vaporization rate were attained at a specific time from ignition. The downward flow of fuel vapor promotes the heat transfer to the liquid surface and increases the vaporization rate, and the liquid flow near the surface is conceivably induced by the outward fuel vapor flow, which is caused by the downward flow.

Paper ID: 147

Characteristics of a blue whirl influenced by different formation conditions

Yifan Yang (Shanghai Jiao Tong University), Haodong Zhang (Shanghai Jiao Tong University), Xi Xia (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University)

This paper focuses on the characteristics of the blue whirl under different formation conditions. The blue whirl is generated using a forced-ventilation fire whirl apparatus, where the fuel supply rate, the tangential incoming flow rate, and the radial incoming flow rate can be independently adjusted. The results show that the fuel supply rate could change the blue whirl' size without affecting the flame regime. And when the fuel is too rich, the upper diffusion flame gradually turns from blue to yellow. The effect of the tangential flow rate on flame transition is hysteretic, resulting in a new phenomenon of a lifted blue whirl. It is found that the centrifugal effect overwhelms the radial-converging effect only when the ratio of the tangential-to-radial flow rate is greater than a critical value, thereby enabling the formation of the blue whirl. This is physically consistent with a recently proposed formation criterion based on a new swirl number.

Paper ID: 148

Numerical investigation on binary droplet bouncing in gaseous crossflow

Yongjie chen (Shanghai Jiao Tong University), Ying Zhang (Shanghai Jiao Tong University), Yai Bai (Shanghai Jiao Tong University), Chunchun Chu (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University), Xi Xia (Shanghai Jiao Tong University)

The present work numerically investigates the binary droplet bouncing upon head-on collision in a gaseous crossflow. The numerical approach employs the volume-of-fluid method with an adaptive mesh refinement algorithm for capturing the gas-liquid interface. The droplet morphology, movement, energy budget, and acceleration of bouncing droplets are compared with those in a static gas medium, demonstrating a nonnegligible effect of the aerodynamic effect during the droplet bouncing process. Results show that weak gas flow has little effect on droplet morphology, while it significantly affects the droplet's acceleration in the impact direction. It is further concluded that this acceleration is attributed to the aerodynamic effect, which generates a pressure difference between the near- and far- interaction zones on the droplet surface.

Paper ID: 149

Biomedical waste combustion in a small-scale packed bed reactor: an Euler-Euler modelling approach

Shyamal Bhunia (Indian Institute of Technology Bombay), Abdul Kadir Poonawala (Indian Institute of Technology Bombay), Arindrajit Chowdhury (Indian Institute of Technology Bombay), Neeraj R Kumbhakarna (Indian Institute of Technology Bombay)

Effective and environment-friendly disposal of biomedical waste (BMW) is essential for the sustainable development of humankind. Though centralized disposal of BMW is encouraged, in-situ processing also demands significant attention. Modelling packed bed combustion is challenging and remains an active research problem. The Euler- Euler modelling approach considering a primary phase (gaseous mixture) and a secondary phase (solid biomedical waste), has been employed in the model development for the packed bed combustor. Heterogeneous reactions, namely moisture removal, waste devolatilization, and char combustion, are considered. Devolatilization significantly impacts mass degradation and flame temperature since the surrogate sample contains a high proximate volatile matter content of 79.29%. Global volumetric reactions like CO, CO_2, H_2, CH_4 and tar oxidation are involved in the gas phase. A good agreement between the experimentally measured temperature profiles and model predictions has been observed. Model-predicted phasic properties and interactions, reaction rates, species concentrations, and flame and bed temperatures convey significant insights into the physics of fixed-bed BMW combustion. More chemical reactions can be incorporated into the physics setup to explore the pollutant formation (NO_x, SO_x etc.) and their pathway at varying O_2 concentrations.

Paper ID: 150

Effect of ultrafine oxygen bubbles on spray combustion

Naoki Hayashi (Kanagawa Institute of Technology), Yusei Akai (Nagoya University), Kazuhiro Yamamoto (Nagoya University)

In this paper, the numerical simulation of spray combustion with ultrafine oxygen bubbles was conducted. It is assumed that oxygen is dissolved in the fuel droplets in the form of ultrafine bubbles (UFB), and released into air when the fuel of decane evaporates. We mainly focus on the chemical effects of UFB on the reaction rate due to the change in oxygen concentration. The evaporation of the fuel droplets was described by a particle-source-in cell (PSI-CELL) model, and the motion of the fuel droplet was also considered. We changed the oxygen concentration in the fuel droplets to discuss the ignition time and the temperature field. As a result, the flame temperature increases and the ignition time is shortened as the concentration of oxygen addition in the droplets increases because the oxygen in UFB addition causes the formation of premixture. The initial droplet diameter and the number of injected droplets per unit time are important parameters for discussing the ignition time and the maximum temperature.

Paper ID: 151

Prediction of ignition modes in shock tubes

Minh Bau Luong (King Abdullah University of Science and Technology), Jiabo Zhang (King Abdullah University of Science and Technology), Miguel Figueroa-Labastida (King Abdullah University of Science and Technology), Aamir Farooq (King Abdullah University of Science and Technology), Hong G Im (King

Abdullah University of Science and Technology)

This study revises the Sankaran number to identify different ignition modes in shock tubes. The non-ideal temperature and pressure rise inherently occurring in shock tubes is incorporated into the predictive criterion. A linear time-varying pressure and the isentropic temperature and pressure relation are assumed to model the temperature and pressure rise, *dT/dt* and *dP/dt*, respectively such that the ignition delay time and the corresponding sensitivity to temperature variation are computed under the shock tube conditions. The Sa_p criterion is then validated by experimental data for a number of fuels exhibiting negative temperature coefficient (NTC) and non-NTC behavior. It is demonstrated that the Sa_p criterion serves as a reliably predictive criterion that can accurately delineate the weak ($Sa_p > 1$) and strong ($Sa_p < 1$) combustion modes regardless of the NTC and non-NTC fuels over a wide range of pressure and temperature. The formulation of the Sa_p criterion also suggests that the sensitivity of ignition delay variation due to the facility-dependent effects such as the polytropic compression/expansion heating effect in a rapid compression machine (RCM) and in an internal combustion engine should be considered for a better prediction of different ignition modes.

Paper ID: 152

Effect of boundary material and fuel pan size on flashover occurrence and energy distribution in compartment fires

Ting Xia (University of Science and Technology of China), Hongli Ruan (University of Science and Technology of China), Yu Wang (University of Science and Technology of China)

Buildings with different walls/ceilings may present different burning characteristics, which normally raises the difficulty of fire development and spread predictions. In this work, to investigate the mechanism of the influence of boundary conditions on compartment fire dynamics, a total of 54 bench-scale experiments with one quarter dimension of ISO 9705 were conducted with three boundary materials and six sizes of fuel pan. Parameters such as the mass loss rate of fuel, the temperatures of the gas, wall and ceiling were measured. It was found that flashover was more likely to occur in compartment of rock wool sandwich panels than in the other two boundaries, but the occurrence of flashover in the compartment of the calcium silicate panels was the last. Moreover, compartments consisting of high thermal conductivity material (corrugated steel sheet) show higher heat loss from the surface to the environment; for the boundary of the high thermal insulation material (calcium silicate board or rock wool sandwich plate), there are few heat losses to the ambient environment (less than 5%) due to low outside surface temperature, while the proportion of heat absorbed by the wall/ceilings is large, with its maximum value even exceeding 30% of the total heat released by fuel. The heat transfer mechanisms of the compartments with different boundary materials were revealed and predicted based on the energy distributions at the transient state in the compartments.

Paper ID: 153

Comparison of effects of H_2 and CH_4 on NH_3 combustion in air: a reactive molecular dynamics study

Jing Wang (Northeastern University), Xi Zhuo Jiang (Northeastern University)

Ammonia is a promising substitute for fossil fuels to achieve the net-zero carbon goals. However, such a sustainable fuel is not easily combustible; to increase the flammability of ammonia, reactive fuels, like hydrogen and methane, is usually added in ammonia combustion. In the present study, comparisons of effects

of CH_4 and H_2 on ammonia combustion were conducted using the reactive molecular dynamics method. The effects of temperature on NH_3/CH_4 and NH_3/H_2 combustion in air were compared. Both H_2 and CH_4 can accelerate the reaction rate of NH_3, and the acceleration by H_2 is more significant than its CH_4 counterpart. The numbers of NO and NO_2 molecules under different temperatures were counted. However, the effects of temperature in both combustions are nonlinear, which requires further exploration of reaction mechanism. The effects of CH_4 and H_2 on combustion intermediates also were discussed. Common and unique intermediates were identified: HN_3, HNO_3 and N_2O_2 were observed in the combustion of NH_3/CH_4, and N_3 is only observed in the combustion of NH_3/H_2. In future work, reaction channels will be explored to elucidate the different effects of H_2 and NH_3 addition on ammonia combustion.

Paper ID: 155

Speed of a flame spreading over a methane hydrate surface

Otabek Nigmatov (Uzbek-Japan Innovation Centre of Youth), Tishihisa Ueda (Teikyo University), Shinnosuke Nishiki (Teikyo University), Oksana Ismailova (Uzbek-Japan Innovation Centre of Youth)

The methane hydrate is expected to be an energy source and a medium for the transportation of natural gases over short and long distances. It is expected to be a transport medium of natural gas alternative to Liquefied Natural Gas(LNG). During transportation using ships and tank trucks, fire accidents are a concern because methane hydrate is combustible. Flame spreading over a methane hydrate surface is studied numerically as a function of a hydrate surface temperature T_s. When T_s = 203 and 213 K, which is the same or higher than the dissociation temperature, T_d, which is 203 K, the flame spreading speed is predicted around 900 mm/s, using the pre-exponential factor 1.90×10^{19} kg/(m^{3}s), which is almost the same as the experimental results. It suggests that the pre-exponential factor changes from 5.44×10^{21} kg/(m^{3}s) to 1.90×10^{19} kg/(m^{3}s) when T_s changes from $T_s < T_d$ to $T_s \geq T_d$.

Paper ID: 156

Effect of ammonia co-firing in 550 MWe USC CFB boiler using CPFD simulation

Yoon-Ho Bae (Pusan National University), Byoung-Hwa Lee (Pusan National University), Min-Woo Kim (Pusan National University), Chung-Hwan Jeon (Pusan National University)

To reduce carbon dioxide in a 550 MWe ultra-supercritical (USC) circulating fluidized bed (CFB) boiler, ammonia co-firing simulation by Computational Particle Fluid Dynamics (CPFD) and its effects are investigated. 10% of the fuel was replaced by ammonia on a lower calorific value basis, and there was no significant difference in boiler internal temperature and heat transfer depending on the injection location. However, significant differences occurred in ammonia slip and N_2O emissions depending on the injection location. This can affect boiler efficiency and N_2O greenhouse effect as co-firing rate increases and needs further optimization. The modeling developed in this study is the first ammonia co-firing simulation conducted for the industrial scale CFB boiler, and the model can be applied to actual technology development in the future.

Paper ID: 157

Comprehensive review on combustion and NOx emission for NH_3 co-firing technology in coal fired power generation

Byoung-Hwa Lee (Pusan National University), Yoon-Ho Bae (Pusan National University), Si-Hyun Cho (Pusan National University), Chung-Hwan Jeon (Pusan National University)

Recently, ammonia has attracted more attention in terms of global carbon neutrality. In order to achieve zero carbon emissions in coal fired power generation, it is most important to replace existing fuels. As a carbon-free fuel, ammonia has several advantages over hydrogen. However, the low burning velocity and high fuel NOx emission of ammonia fuel are challenges in practical use. Therefore, in this paper, ammonia fuel was first analyzed and reviewed in terms of thermal properties and fundamental combustion characteristics. This paper also evaluates and discusses the mechanisms of NOx emissions that can be rapidly elevated by NH_3. Based on the reaction mechanism, the characteristics of major NOx production and reduction under various conditions were identified and several methods for NOx control were presented. In particular, it contributes to finding optimal conditions by analyzing the ammonia co-firing characteristics of existing coal-fired boilers. This study systematically summarizes the basic combustion behavior of ammonia fuel and uses it as a theoretical reference for ammonia combustion and exhaust emissions to suggest practical applications in power generation fields where ammonia conversion is important.

Paper ID: 158

Chemical structure effect on agglomeration and combustion characteristic of high volatile coals in blast furnace

Min-Woo Kim (Pusan National University), Jang-Ho Jo (University of Newcastle), Dae-Gyun Lee (Pusan National University), Byoung-Hwa Lee (Pusan National University), Chung-Hwan Jeon (Pusan National University)

In the blast furnace, pulverized coal injection (PCI) system used for reduction of operation cost by injecting directly thermal coal instead of bituminous coal. The increase in the use of high volatile coals (HVCs) is inevitable in terms of fuel supply and cost. In this study, the relation between combustibility and agglomeration of HVCs due to chemical structure effect is investigated using drop tube furnace (DTF) and attenuated total reflectance Fourier transform infrared (ATR FT-IR) analysis. DTF is used for combustibility and agglomeration experiments. The char collected by DTF experiments was analyzed for combustibility by measuring unburned carbon (UBC). Also, agglomeration ratio was analyzed using the mass ratio of agglomerates in char. The IR spectrum of each sample was analyzed using ATR FT-IR, and Aromatic carbon fraction (Fa) and aliphatic CH_2/CH_3 ratio was analyzed. The combustion characteristics and chemical structure effect on agglomeration of HVC used in the blast furnace were investigated by DTF experiment and ATR FT-IR analysis. It is found that agglomeration increase the particle size and decrease combustibility, and agglomeration is affected by aliphatic hydrocarbons.

Paper ID: 159

Effects of gas compositions on NOx formation during char combustion in waste incineration

Ryo Yoshiie (Nagoya University), Kazutaka Tsukamoto (Nagoya University), Yasuaki Ueki (Nagoya University), Ichiro Naruse (Nagoya University), Taichi Usuki (JFE Engineering Corporation), Tomohiro Denda (JFE Engineering Corporation)

An incineration process is the most dominant method of the waste disposal in Japan. Stoker boilers are widely used for the waste incineration. In the stoker furnace incinerator, waste products can be sufficiently stirred and burned completely. Recently, low air ratio and high temperature incinerations have been applied to the stoke furnace incinerator to improve efficiencies of power generations. However, these operation conditions cause the increase in NOx emission due to higher flame temperatures. In addition, Exhaust Gas Recirculation (EGR) system, which is also applied into advanced incinerators, makes the NOx formation more complicated. In this research, NOx and other gaseous emissions from RDF char combustion were experimentally analyzed, investigating effects of exhaust gas compositions on NOx formations.

Paper ID: 160

Enhancement of ammonia auto-ignition with low-carbon fuels: multi-species time history measurements and kinetics modeling

Jiabiao Zou (KAUST), Mohammad Adil (KAUST), Ali Elkhazraji (KAUST), Aamir Farooq (KAUST)

A comprehensive laser absorption diagnostics system was constructed to measure NH_3, NO, N_2O, H_2O, and CO in neat NH_3, NH_3/CO, NH_3/H_2, and NH_3/CH_4 dual-fuel oxidation behind reflected shock waves over 1201-2271 K, 1.02-2.04 bar and $0.5 < \phi < 1.0$. A comprehensive kinetic model containing NH_3, NH_3/H_2, NH_3/CO, and NH_3/CH_4 oxidation mechanisms was constructed to explore the enhancement effects of H_2/CO/CH_4 for NH_3 auto-ignition and NOx formation. We found that the branching step $H+O_2=OH+O$ in H_2/O_2 system dominates fuel consumption and NOx formation. In the case without fuel-H_2, H-abstraction of NH_i can act as an H_2 source for H_2/O_2 system. The replacement of NH_3 with H_2 can enhance the reactivity of H_2/O_2 chemistry and result in much shorter IDTs in NH_3/H_2 system, while the replacement with CO and CH_4 only slightly enhances the ignition process. Moreover, the replacement of NH_3 with CH_4 can significantly enhance O formation and heat release, which can further enhance NOx formation. Finally, the replacement of CO with NH_3 can only do minor enhancement of NH_3 ignition and oxidation, but can significantly inhibit NO formation under lean conditions.

Paper ID: 161

An experimental study of direct iron ore reduction using ammonia

Zhezi Zhang (The University of Western Australia), Chiemeka Okoye (The University of Western Australia), Darren Matthews (Rio Tinto), Dongke Zhang (University of Western Australia)

This paper reports an experimental study of the effects of reduction temperature and gas flowrate on a hematite-goethite iron ore using NH_3. The ore sample was reduced in 20% NH_3/Ar for various durations in a fixed-bed reactor at 450°C, 600°C, 900°C and 1050°C. The mineralogical compositions of the raw and reduced samples were characterised using XRD. Weight loss and degree of metallisation were calculated. Flue gas composition was analysed using a GC, NOx analyser and FTIR. Wustite and Fayalite were found to be

the primary intermediates during the transformation of the iron oxides to metallic iron. Analysis of the flue gas showed that at high temperatures (900°C and 1050°C) NO can form early in the experiments from reaction of NH_3 with the iron ore. It is also believed that metallic iron catalyses the dissociation of NH_3 supporting the continued ore reduction by H_2.

Paper ID: 162

Hygrothermal aging of Magnesium particles and performance of metal-fluorocarbon pyrolants

Juyoung Oh (Seoul National Univ Korea), Yejun Lee (Seoul National University), Jack J. Yoh (Seoul National Univ Korea)

Magnesium (Mg) powders have been widely utilized in space power systems and recently have been paid attention as a renewable energy carrier. However, for the long-term usage of Mg-related energetic materials, hygrothermal aging effects should be addressed in advance as Mg particles are highly reactive to moisture. The present study for the first time found hygrothermal aging effects on Mg particles and identified their influence in MTV igniters which have not been reported yet. Thermal analysis was conducted to observe the changes in the thermochemical characteristics of both Mg particles and Magnesium/Teflon/Viton (MTV) granules under hygrothermal aging. Morphological changes due to aging were explained via surface analysis. It is observed that the hygrothermally aged Mg powders easily reacted with H_2O and formed $Mg(OH)_2$ and MgO layers outside. For hygrothermally aged MTV igniters, the amount of decomposed $Mg(OH)_2$ during the combustion increased proportionally to the relative humidity levels indicating that Mg within the compounds can be still reactive to the moisture. Comprehensively, thermal aging affected the changes in reaction paths of the vapor phase combustion of MTV igniters while hygrothermal aging gave rise to the degradation in both the condensed and the vapor phase combustion of MTV.

Paper ID: 163

A reduced chemical kinetic mechanism for ammonia combustion targeted on multiple prediction objectives

Huaiyin Wang (Tianjin University), Tianyou Wang (Tianjin University), Ming Jia (Dalian University of Technology), Zhen Lu (Tianjin University), Yachao Chang (Dalian University of Technology), Kai Sun (Tianjin University)

In this work, a reduced ammonia kinetic model was developed to achieve a comprehensive prediction performance of ammonia combustion. The method of the comprehensive reduced mechanism construction based on multiple objectives, i.e., ignition delay time (IDT), laminar flame speed (LFS), and species concentrations, was proposed. Three detailed mechanisms are firstly identified to best predict the IDT, LFS, and species concentration, respectively. The species-based path sensitivity analysis (PSA) and global sensitivity analysis (GSA) were utilized to identify the species importance of the specific detailed mechanisms. Three interim reduced mechanisms were attained by eliminating the redundant species until the relative error between the predicted results using the interim reduced mechanisms and the detailed mechanisms exceeded error limit. An initial comprehensive mechanism was constructed by coupling the three reduced mechanisms. The rate constants of the dominant reactions in the ammonia sub-mechanism were optimized under the uncertainty of reaction rates through a multi-objective optimization method to improve the prediction

performance. Overall, the current kinetic model can predict well IDTs, LFSs, and species concentrations of ammonia over a wide range of experimental conditions.

Paper ID: 164

Validation of a reactive flow solver based on OpenFOAM for detonation modeling

Vigneshwaran Sankar (KAUST), Karl P. Chatelain (KAUST), Josue Melguizo-Gavilanes (Centre National de la Recherche Scientifique), Deanna Lacoste (KAUST)

An OpenFOAM (OF) based hybrid reacting flow solver is developed and validated to compute detonation waves. This solver is developed by incorporating the features of standard OF solvers viz., rhoCentralFoam, reactingFoam, and pimpleFoam. The hybrid implementation is a feature that allows for efficient computation of deflagration to detonation transition (DDT) where we switch between numerical schemes that are suitable for Mach number (M) < 0.3 (i.e PISO/SIMPLE) and typical flux splitting/limiters for high speed regimes with discontinuities. For the case at hand, only the latter is active. The solver performance is verified and validated with one- (1D) and two-dimensional (2D) simulations in both laboratory- (LFR) and shock-attached (SFR) frame of reference for a stoichiometric H_2-O_2-Ar mixture at low pressure. First, the results obtained from LFR simulations were compared against ZND solutions and are in good agreement on an average sense. Second, 2D SFR simulations were performed and validated for a more efficient use of the computational capacity. We found that at least 24 points per induction zone length is required to resolve the 2D detonation structures for the present SFR simulation. Also, the detonation cell width (λ) obtained from numerical smoke foils are in good agreement with reported detailed chemistry simulations.

Paper ID: 165

Large eddy simulations of hydrogen/ammonia bluff-body flames

Suliman Abdelwahid (KAUST), Francisco E. Hernández-Pérez (KAUST), Adamu Alfazazi (King Abdullah University of Science and Technology), Ayman Elbaz (KAUST), Jiajun Li (KAUST), Bassam Dally (KAUST), Hong G. Im (KAUST)

Ammonia (NH_3) is a hydrogen carrier and, as a fuel, has been proposed as an alternative to fossil-based fuels in order to curb the influence of CO_2-emission on global warming. Ammonia has been traded for a long time and well-developed systems to store, deliver, utilize, and convert it back into its main constituents, nitrogen and hydrogen, are in existence for many decades. However, one of the main issues associated with NH_3 combustion is its relatively low reactivity compared to conventional fuels. One technique for boosting NH_3 reactivity is to pre-crack it into H_2-containing mixtures (H_2/N_2) before introducing it into combustion systems. To reduce the cost and the need for pre-cracking of the fuel, recirculation zones that are induced in bluff-body burners can function as an in-situ cracker region for NH_3 flames. To achieve this, numerical and experimental investigations are required. This study aims at investigating the fundamental characteristics of NH_3/H_2/N_2 non-premixed bluff-body stabilized flames and assess flamelet-based models by contrasting their large eddy simulation (LES) predictions against recent measurements obtained at KAUST. Two turbulent (Re~5500) flames are investigated, FNH_3_0 (75% H_2:25%N_2 by vol.) and FNH_3_72 (72%NH_3:21% H_2:7%N_2 by vol.). The comparisons showed that the LES successfully reproduced the global flame characteristics with reasonable accuracy including the extinction phenomena.

Paper ID: 166

An evaluation of micro-mixing models in transported pdf simulations of a hydrogen flame with strong thermodiffusive instabilities

Xiao Wang (Tsinghua University), Tianwei Yang (Tsinghua University), Lukas Berger (RWTH Aachen University), Heinz Pitsch (RWTH Aachen University), Hua Zhou (Tsinghua University), Zhuyin Ren (Tsinghua University)

Utilizing hydrogen as a fuel is a promising option for a carbon-neutral industry. However, a variety of problems could emerge when burning hydrogen, especially under lean premixed conditions, e.g., hydrogen flames are prone to thermodiffusive instabilities. In this work, TPDF simulations are performed to compare against a DNS dataset of a lean premixed turbulent hydrogen/air flame to evaluate the micro-mixing models and mixing timescales. The TPDF simulation applies the same chemical kinetics as the DNS, and employs the DNS-extracted mean velocity, turbulent diffusivity and turbulence frequency, enabling a rigorous evaluation of the micro-mixing effects. The study demonstrates that the TPDF simulation exhibits large sensitivity to the micro-mixing model. The TPDF simulation could reasonably predict the flame length indicated by the centerline temperature when the EMST model is employed with C_ϕ = 5. As far as the mixing timescale is concerned, increasing C_ϕ enhances the overall combustion progress regardless of the micro-mixing models, and the MC model requires a larger C_ϕ to yield a similar prediction as the EMST model. This study shows that the TPDF simulation with a single mixing timescale fails to reproduce the key features of thermodiffusive instabilities, e.g., super-adiabatic temperatures, and therefore, constructing micro-mixing models which accounts for the differential mixing could be essential for flames of this kind.

Paper ID: 168

Turbulent non-premixed combustion of pyrolysis gas in a swirl burner

Nana QI (North China Electric Power University), Long Yan (North China Electric Power University), Zhezi Zhang (The University of Western Australia), Dongke Zhang (University of Western Australia), Kai Zhang (North China Electric Power University)

A numerical analysis of the combustion of pyrolysis gas and associated NOx emission characteristics is conducted in a burner with swirl primary air injectors. A comprehensive model is established by involving the nonlinear second-moment turbulence model, discrete transfer radiation model, eddy dissipation combustion model and a comprehensive reaction mechanism. The numerical simulation results show that the swirl vane improves the uniformity of temperature distribution of the flame, significantly enhances the combustion efficiency of the pyrolysis gas, and dramatically reduces the NO emission by controlling the internal recirculation flow structure. In addition, the primary air coefficient has a complex effect on NO emission as the turbulent flow structure is complicated in the central combustion region. NO concentration is first increased and then decreased with the increasing the primary air coefficient.

Paper ID: 169

Effects of aluminum oxide nano-particulate additives on energy performance and emission characteristics of diesel engine at various excess air coefficients

Zhefeng Guo (Beijing Institute of Technology), Sheng-Lun Lin (Beijing Institute of Technology)

This experimental study is mainly about the energy performance and emission characteristics of a single-cylinder diesel engine fueled with diesel containing aluminum oxide nanoparticles. In this study, tested fuels with added concentrations of 50 and 100 ppm were prepared using ultrasonic technique and surfactant Span-80. Then fuel combustion tests were performed at different excess air coefficients (1.4, 1.6, 1.8, 2.0) at the maximum torque speed of 1800 rpm. The results showed that the addition of nanoparticles did not significantly affect the BSFC and BTE of DEs. However, the SOOT-NOx-PM emission trade-off in previous studies has been overcome by using added aluminum oxide nanoparticles due to better fuel atomization and uniform and complete combustion. Notably, the addition of aluminum oxide nanoparticles caused a surge in the number of ultra-fine and fine particles with health hazards when the DEs was operated at an excess air coefficient value is 2.0.

Paper ID: 170

On the laminar flame speed of gasoline-air mixtures with reaction progress

Haruki Tajima (Keio University), Takuya Tomidokoro (Keio University), Takeshi Yokomori (Keio University)

Understanding flame propagation in a partially-reacted fuel-air mixture is necessary to prevent knocking in spark-ignition (SI) engines. Regarding the influence of reaction progress on the laminar flame speed SL, previous studies have focused on low temperature chemistry (LTC) and examined its effect on temperature and chemical composition of the mixture. However, the influence of pressure increase caused by reaction progress has not been considered. This study investigates SL in partially reacted gasoline-air mixtures under different initial temperatures, pressures, and excess-air ratios. Two reactors in ANSYS Chemkin-Pro software were coupled. The first reactor simulates a homogeneous isochoric reaction progress for a finite residence time. Then, the output of the first reactor was used as the inlet condition of the second reactor, which simulates a steady one-dimensional planar flame propagation. In all cases, SL was increased when reaction progress was given. The LTC in the homogeneous reactor modified the temperature, pressure, and chemical composition of the mixture. This altered the thermal and chemical structure of the flame compared to the flame with no reaction progress.

Paper ID: 171

Direct observation of reactive intermediates in the catalytic partial oxidation of iso-octane on nickel

Jijun Guo (Shanghai Jiao Tong University), Zaili Xiong (Shanghai Jiao Tong University), Yuwen Deng (SJTU), Bingzhi Wang (University of Science and Technology of China), Hao Lou (University of Science and Technology of China), Meirong Zeng (Shanghai Jiao Tong University), Zhandong Wang (University of Science and Technology of China), Zhongyue Zhou (Shanghai Jiao Tong University), Wenhao Yuan (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University)

Catalytic partial oxidation (CPO) of petroleum-based alkanes is an efficient method to produce syngas (H_2/CO), which is cleaner energy used in engine or chemical industry. Comprehensive probing of the species pool is essential to reveal the role of homogenous and heterogenous chemistry during the CPO process. In this work we reported a comprehensive experimental investigation on the CPO of iso-octane on silica-supported Ni catalyst. The experiments were carried out in a packed bed flow reactor at the pressure of 0.1 atm and temperature range 573-973 K. Synchrotron vacuum ultraviolet photoionization mass spectrometry (SVUV-

PIMS) was used to detect and identify the CPO products. Dozens of products were detected, including radicals like vinyl radical, ethyl radical, methoxy radical, allyl radical, as well as isomers like allene and propyne. The experimental results provide an overall view on the gas-phase reaction network during the CPO of iso-octane.

Paper ID: 173

Analysis of flame dynamics in a stratified swirl burner using spectral proper orthogonal decomposition

Junhua Zhang (Beihang University), Qiang An (Beihang University), Zhipeng Yang (Beihang University), Xin Hui (Beihang University), Xiao Han (Beihang University)

Stratified swirl burners, featuring a combination of inner and outer swirlers separated by a lip structure, are widely employed to achieve low pollutant emissions. This paper experimentally investigates the flame shapes and corresponding dynamics as a function of stratification ratio SR, defined as the ratio of the inner equivalence ratio to the outer equivalence ratio, and outer-stage swirl numbers S in a stratified swirl burner. Depending on the specific SR and S, four distinctive flame shapes are observed, i.e. a lifted flame, an attached V-flame, an attached M-flame, and an attached M-flame surrounded by an attached V-flame. Spectral proper orthogonal decomposition (SPOD) is then used to analyze the flame dynamics. The results show that the flame dynamics are mainly dominated by broadband turbulent vortices for high values of S with all SR, whereas large-scale coherent structures are observed in the flames for low values of S with high SR. Further analysis found that these coherent fluctuations mainly take place in the inner flame and are driven by the axisymmetric and helical vortices, whereas increasing S or decreasing SR suppresses these fluctuations.

Paper ID: 175

Thermodynamic and economic analysis of a conceptual system combining sludge gasification, SOFC, supercritical CO_2 cycle, and organic Rankine cycle

Jiayang Lv (North China Electric Power University), Heng Chen (North China Electric Power University), Kai Zhang (North China Electric Power University), Guoqiang Zhang (North China Electric Power University), Dongke Zhang (University of Western Australia)

In order to reduce the environmental impact of conventional sludge treatment and to utilize the energy in sludge more effectively, a coupled system based on sewage sludge gasifier (SSG), solid oxide fuel cells (SOFC), supercritical CO_2 cycle (S-CO_2), and organic Rankine cycle (ORC) is proposed. The clean syngas obtained from sludge gasification is mixed with CH_4 and then first utilized by the fuel cell. The exhaust gas from the fuel cell is fully combusted in the afterburning chamber and then enters the bottom cycle system consisting of S-CO_2 & ORC to generate electricity. In order to further understand the system performance, the thermodynamic and economic analysis of the system was carried out. It was found that the proposed system could achieve a net output of 37.34 MW with a net efficiency of 64.45%. It takes only 6.13 years to repay the construction investment in the proposed system, and the project obtains a net present value of 17723.82k$ during 20 years lifetime. The conclusions show that the project is advantageous and beneficial in sludge waste utilization.

Paper ID: 176

The effects of NH_3 addition on the morphology and nanostructure of soot particles in laminar diffusion n-decane flames

Zhiyu Yan (Xi'an Jiaotong University), Tianyi Zhu (Xi'an Jiaotong University), Qianqian Li (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University)

In order to evaluate the effects of NH_3 addition on soot formation in laminar diffusion kerosene surrogate flames, the thermophoresis sampling method was used to study the particle evolution of the morphology and nanostructure. The flame of Ar addition was set as dilution case to be compared. The results show that the flame height increases significantly when NH_3 is doped, and the increase of pyrolysis region means the soot formation is delayed. The transmission electron microscope (TEM) images show that the particle nucleation can be inhibited, and the aggregate sizes are smaller in NH_3-$C_{10}H_{22}$ flame. Compared with the Ar addition flame, doping NH_3 into the n-decane flame reduces the primary particle diameter more obviously, which means that chemical effect can suppress the particle surface growth. At HAB of 40 mm, although the particle graphitization occurs in all three flames, the proportion of short lattice fringes rises in the NH_3 rich flame. This means particles can be oxidized more easily. These results have the significance for the particle control in the aviation field.

Paper ID: 177

Flickering buoyant diffusion flames in rotatory flows

Tao Yang (The Hong Kong Polytechnic University), Peng Zhang (City University of Hong Kong)

Flickering buoyant diffusion flames in rotatory flows are investigated with emphasis on the flame dynamical behaviors in a large rotatory intension range. Diffusion flames are produced computationally and imposed in different rotatory flows, which are generated by four wing walls. In a quiescent environment, the flicker frequency follows a scaling law of $f\sim\sqrt{(g/D)}$. With the rotatory intensity R enhancing, the buoyancy-induced oscillation becomes faster at first and vanishes finally. In the weakly rotatory flow, the increase of f obeys the scaling relation $(f-f_0)\propto R^{\wedge 2}$, which agrees very well with the present computational results. When R is large, the local extinction occurs at the flame base and the flame lifts off. In the present study, six distinct flame modes including flickering, oscillating, steady, spiral, lifted, and vortex-bubble flames are found in the various rotatory conditions. Based on the understanding that phase portraits are an invaluable tool in studying dynamical systems, different flame modes are illustrated in phase space.

Paper ID: 178

On the relationship between displacement speed and curvature in hydrogen/methane premixed flames

Jen Zen Ho (The University of Melbourne), Mohsen Talei (The University of Melbourne)

Direct Numerical Simulation (DNS) of four turbulent premixed jet flames with a bulk Reynolds number of 10,300 fuelled with 0/100, 10/90, 50/50 and 80/20% H_2 / CH_4 by volume are studied. The Markstein lengths relating displacement speed with curvature are found to decrease as hydrogen content increases and have different values for positive and negative curvatures. In addition, the density-weighted displacement speed is found to be related to the curvature by a flame thickness and the contribution of the reaction, normal and tangential diffusion terms to the displacement speed is found.

Paper ID: 179

Experimental study of droplet collision under weak air crossflow

Yai Bai (Shanghai Jiao Tong University), Yongjie chen (Shanghai Jiao Tong University), Dawei Zhang (Shanghai Jiao Tong University), Chunchun Chu (Shanghai Jiao Tong University), Ying Zhang (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University), Xi Xia (Shanghai Jiao Tong University)

This paper reports an experimental study of the collision dynamics of binary water droplets under weak air crossflow, with an emphasis on exploring the aerodynamic effects. The collision outcomes for the cases with and without crossflow are compared in the classical collision regime diagram of Weber number vs. impact parameter, showing a negligible effect of the aerodynamic effect for the present study. The droplet collision process is further divided into the compression, stretching, and retraction stages based on the evolutions of the droplet's maximum and minimum dimensions. Applying an energy budget analysis, we find that the aerodynamic force acts on the compression stage by preventing drop spreading, further resulting in increased energy dissipation.

Paper ID: 180

Kinetic study of plasma-assisted low-temperature oxidation of ammonia

Haodong Chen (Tsinghua University), Zhongkai Liu (Tsinghua University), Zhaoying Li (Tsinghua University), Bin Yang (Tsinghua University)

The chemical kinetics of low-temperature oxidation of ammonia (~340 K, 30 Torr) activated by a nanosecond discharge is explored by electron-ionization molecular beam mass spectrometry (EI-MBMS) and kinetic modeling. Species mole fractions are measured under different oxygen concentrations and peak voltages. The fuel consumption and the formation of NO and N_2O are enhanced by the increase of the O_2 contents and peak voltages under the present experimental conditions. The non-monotonic profile of N_2 mole fractions under different O_2 concentrations indicates a competition between the oxidative pathway and non-oxidative pathway leading to its formation. A kinetic mechanism consisting of plasma and low-temperature oxidation reactions is developed. Most of the species detected in the experiments are well-predicted by the model. The pathway fluxes of the fuel consumption and subsequent reactions are displayed based on the rate of production (ROP) analysis. In fuel-rich cases, the NH_2 recombination pathway forming N_2H_4 is emphasized, which only plays a minor role in fuel-lean cases. The incomplete description of reactions involving electronically excited O_2 and electronically excited O may account for the underestimation of the N_2O.

Paper ID: 181

Breakup and lifting of a falling droplet in air crossflow

Chunchun Chu (Shanghai Jiao Tong University), Yongjie chen (Shanghai jiao tong university), Yai Bai (Shanghai Jiao Tong University), Ying Zhang (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University), Xi Xia (Shanghai Jiao Tong University)

In the present study, the deformation and secondary breakup of a single droplet in air crossflow are experimentally investigated in a small-size wind tunnel. By tuning the initial droplet diameter, droplet falling height, and crossflow velocity, we obtain various droplet deformation and breakup modes, which are presented in the regime diagram involving the gas-phase and liquid-phase Webber numbers. Furthermore, a unique

droplet lifting phenomenon is found in the deformation mode. The underlying lift mechanism can be attributed to the formation of an oblique windward, which has been shown to lead to the deflection of the drag force on the droplet. The upward component of this drag gives rise to a substantial lift which significantly overweighs the droplet's weight, resulting in the vertical deceleration of the droplet and then an abrupt upward turning in its trajectory.

Paper ID: 182

Multilevel characterization scheme for confined turbulent diffusion flames

Assiz M P (LPSC ISRO), Debi Prasad Mishra (NITTTR Kolkata, IIT Kanpur)

Turbulent diffusion flames commonly exist in propulsion systems and industrial combustors. Characterization schemes for a confined turbulent diffusion flame are presented at two different levels. Characterization by means of flame length is followed at the first level. Evaluation of the flame length is carried out by applying a novel 'Image Processing Technique (IPT)'. The characteristic flame lengths Total Flame Length (TFL) and Bluish Flame Length (BFL) are introduced. In the second level, a performance parameter (BT ratio) is evolved to characterize the flame. These two parameters describe a turbulent diffusion flame in a combustor at a given confinement ratio. A swirl coaxial injector is used to inject the propellants (methane and oxygen) into a quartz tube combustor. Experiments using a Bunsen burner, and invoking associated hypotheses, show that the performance parameter of the flame (BT ratio) carries the signature of combustion efficiency for a particular injector-combustor configuration at a given operating condition.

Paper ID: 183

Large-eddy simulation of a natural gas DISI engine: effects of laminar and turbulent flame speed modelling

Mohammadreza Yosri (The University of Melbourne), Mohsen Talei (The University of Melbourne), Robert Gordon (The University of Melbourne), Michael Brear (The University of Melbourne)

Large-Eddy Simulation (LES) of a Compressed Natural Gas Direct Injection Spark Ignition (CNG DISI) engine is performed using the G-Equation approach. Flame propagation features two stages: in the first stage the flame propagates like a laminar flame until it reaches a certain cut-off radius whereas in the second stage, the flame is turbulent. Three different laminar flame speed correlations and three different turbulent flame speed models are tested in this transition model. Changing the laminar flame speed correlation greatly affects the transition time and consequently the pressure trace and the Mass Fraction Burned (MFB) profile. The Reyes et al. laminar flame speed correlation gives the best performance amongst all with the cut-off radius used in the literature. However, for the other laminar flame speed correlations, the cut-off radius needs to be tuned to obtain a good agreement. Furthermore, where the Reyes et al. correlation is used, the constants for the turbulent flame speed models of Muppala et al. and Kobayashi et al. need to be tuned to obtain reasonable results whereas the Damköhler model works well with the constant reported in the literature. In conclusion, the findings of this study show that the laminar flame speed correlation in conjunction with the turbulent flame speed model need to be carefully selected in LES.

Paper ID: 184

Towards the development of liquid ammonia/air spray combustion in a gas turbine-like combustor

KDKA Somarathne (Tohoku University), H Yamashita (Tohoku University), S Colson (Tohoku University), A Hayakawa (Tohoku University), T Kudo, H Kobayashi (Tohoku University)

Ammonia is already identified as a prominent energy vector in a carbon-neutral society of 2050. This study numerically investigates the emission characteristics of liquid ammonia (LNH_3) spray combustion in a gas turbine-like combustor at 0.3 MPa. LNH_3 contained a higher energy density than gaseous ammonia (GNH_3). LNH_3 is commercially available in high-pressure cylinders approximately at about 0.9 MPa at room temperature. However, pressurized LNH_3 becomes superheated and subsequently resulted in a flashing spray when discharged into a low-pressure environment through a nozzle. Thus, in this study, it was essential to account for the non-equilibrium flash boiling phenomenon in addition to the convective evaporation. On the other than owing to the high latent heat of ammonia, the temperature of the two-phase flashing spray was as lower as -60 °C at 0.1 MPa. Thus, it was essential to use preheated air for flame stabilization. Before obtaining stabilized pure LNH_3/air flames, LNH_3 spray was co-fired with gaseous hydrogen based on ammonia energy fraction in the fuel streams such as 50%, 60%, and 70%, and eventually, emission characteristics were comprehensively studied. Numerical codes were validated using axial and radial temperature measurements of non-reacting LNH_3 spray flow at 0.1 MPa.

Paper ID: 185

Investigation of the flame structure of turbulent ammonia-hydrogen-nitrogen flames by simultaneous NH and NO planar laser-induced fluorescence

Guoqing Wang (King Abdullah University of Science and Technology), William Roberts (KAUST), Thibault Guiberti (KAUST)

Turbulence-chemistry interactions play a key role in determining the stability and emissions of ammonia-hydrogen combustion. The simultaneous NH and NO planar laser-induced fluorescence (PLIF) method, which is one of the most powerful laser diagnostic techniques for measuring different species, was used to study the flame structure of turbulent ammonia-hydrogen-nitrogen non-premixed flames at pressures ranging from 1 to 5 bar and cracking ratios from 7% to 28%. The multi-scalar PLIF method allowed for visualization of the flame morphology. The number of NH-layer fragments, length, and thickness were extracted from NH-PLIF images at different heights. The results showed that NH well marks the heat release layer of the non-premixed flames. The flame surface merge, local extinction, and turbulent mixing significantly influence its thickness. The cracking ratio strongly impacted the chemical reactivity of the ammonia-hydrogen flames, which determines flame stability and NH-layer characteristics. NO is quickly formed within the reaction zone and remains present in the outer hot products until turbulent mixing reduces the NO concentration and temperature.

Paper ID: 186

Onset of flame acceleration in unconfined propane-oxygen mixtures

Akihiro Ueda (Hiroshima University), Keita Tanaka (Hiroshima University), Yangkyun Kim (Korea Institute of Civil Engineering and Building Technology), Wookyung Kim (Hiroshima University)

In this study, the explosion characteristics of propane-oxygen mixtures were investigated experimentally and

numerically. The critical flame radius, the critical Péclet number at which flame acceleration occurs and unstretched laminar burning velocity of the propane-oxygen mixture were investigated using the soap bubble method. Furthermore, the combustions under the experimental conditions were calculated as a steady one-dimensional laminar flame using Chemkin-Pro software and compared with experimental results. The experimental values of unstretched laminar burning velocity and critical Péclet number agreed qualitatively with calculated values, and the critical Péclet number tended to decrease with increasing equivalence ratio. Also, the dependency of Pec on Mab and Mab on Kac for propane-oxygen flame were compared with that for other fuel-air mixtures. The values showed that when the combustion-supporting gas was oxygen, the unstable regime was wide, and the flame became unstable from the initial stage of the flame.

Paper ID: 187

Numerical study of the unsteady drag on a droplet accelerated by a uniform gas flow

Ying Zhang (Shanghai Jiao Tong University), Yongjie chen (Shanghai jiao tong university), Yai Bai (Shanghai Jiao Tong University), Chunchun Chu (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University), Xi Xia (Shanghai Jiao Tong University)

The unsteady drag on a droplet accelerated by a uniform gas flow is investigated numerically using the volume-of-fluid (VOF) method with adaptive mesh refinements. Results show that the unsteady drag fluctuates periodically with droplet deformation. However, the saturated drag coefficient for a stabilized droplet is different from that of an equivalent rigid particle by a constant specific to the Webber number. Furthermore, this drag-coefficient difference shows a decreasing trend with increasing Weber number, which is attributed to the changes in the unsteady effect of the droplet and the wake flow caused by a larger droplet deformation. The understanding obtained from this work could shed some light on the dynamical effect of droplet-gas interaction influenced by aerodynamic force.

Paper ID: 188

Ignition delay time and flame speed validation of a reduced n-dodecane mechanism using a hybrid reduction method

Anurag Dahiya (National Tsing Hua University), Ying-Di Li (National Tsing Hua University), Zi-Jia Wang (National Tsing Hua University), Yun-Jui Wu (National Tsing Hua University), Kuang C. Lin (ASPACC 2023)

n-dodecane is one of the important surrogates of jet fuel. To understand combustion behavior in 0-D, 1-D, and 2-D reactors need to reduce the mechanism with better accuracy. This study proposes a reduced mechanism for n-dodecane by using a hybrid reduction technique. In the first step, a detailed mechanism (255 species and 1521 reactions) is reduced by using path flux analysis (PFA). The reduced mechanism by PFA consists of 128 species and 687 reactions. In the second step, a reduced mechanism by PFA further reduces by an artificial neural network (ANN). The final reduced mechanism using PFA and ANN consists of 94 species and 516 reactions. The reduced mechanism of n-dodecane is well-validated in ignition delay time and flame speed.

Paper ID: 190

Reactive inception model for soot modeling in laminar inverse diffusion flames

Junjun Guo (King Abdullah University of Science and Technology), Peng Liu (King Abdullah University of Science and Technology), Erica Quadarella (King Abdullah University of Science and Technology), William Roberts (KAUST), Hong G. Im (KAUST)

Inception describes the transition from soot precursors to the condensed phase and remains one of the least understood steps in soot formation. While the physical inception model is widely used in soot modeling, our previous study [*Combust Flame 246 (2022) 112420*] showed that it is not able to capture the soot behavior in laminar inverse diffusion flames (IDF). In this study, a simplified reactive inception model is developed, including reversible dimerization for physically-bounded dimer formation, dimer dehydrogenation by H and OH radicals, and chemically-bounded dimer formation. The simulations of IDF show that the predicted soot behaviors agree well with the experiments, which evidences the importance of radical involvement in soot inception process.

Paper ID: 191

Flame-flow dynamic behavior at mode transition during combustion instability in lean premixed low-swirl hydrogen-methane turbulent flames

Takeshi Shoji (Japan Aerospace Exploration Agency), Ryota Fujii (Keio University), Judai Masugi (Keio University), Kentaro Horikawa (Keio University), Shigeru Tachibana (Japan Aerospace Exploration Agency), Takeshi Yokomori (Keio University)

The flame-flow behavior of lean premixed low-swirl H_2-CH_4 turbulent flames was experimentally investigated through simultaneous 10-kHz OH* chemiluminescence imaging, 40-kHz stereoscopic particle image velocimetry, and 200-kHz pressure fluctuation measurements. The mixture bulk velocity and equivalence ratio were fixed at 15 m/s and 0.65, respectively, while the mole fraction of H2 in the blend fuel (α) was varied. The results indicate that, as α gradually increases, the high-frequency (HF) to low-frequency (LF) mode shift of combustion instability (CI) occurs approximately at α = 0.5. At the fixed α of 0.5, corresponding to the transitioning regime, irregular transitions, such as the LF-to-HF or HF-to-LF mode transition, also occur in the CI mode. For the LF-to-HF mode transition, the flame macrostructure does not vary significantly, although the phase relation between the fluctuations in the pressure, unsteady heat release rate, and volume flow rate changes. Additionally, the spectral analysis reveals that the flame periodically extends upstream toward the shear layer region in the frequency range of approximately 20–167 Hz. Dynamic mode decomposition reveals periodically oscillating flame structures around the shear layer region in the same frequency range as in the spectral analysis, which is likely a precursor of the mode transition.

Paper ID: 192

Dynamical modes of triple flickering flames

Yicheng Chi (City University of Hong Kong), Tao Yang (The Hong Kong Polytechnic University), Peng Zhang (City University of Hong Kong)

In the present study, we experimentally studied the triple flickering buoyant diffusion flames, considered a nonlinear dynamical system of coupled oscillators, in an isosceles triangle arrangement. The study includes

three major aspects. First, we established a well-controlled gas-fuel diffusion flame experiment to remedy the deficiencies in previous candle-flame experiments. Then, we developed phase-space-based and Wasserstein-space-based methodologies for dynamical mode recognition, which have been validated in the present study but can be extended to larger dynamical systems. Through the present experiment and proposed methods for dynamical mode recognition of the triple-flame system, we recognized seven distinct stable dynamical modes. Finally, we for first the time established a regime nomogram for the dynamical modes of the triple-flame system. It should be noted that the present study mainly focuses on proposing and validating a relatively objective methodology for dynamical mode recognition, namely from physical space to phase space and then to Wasserstein space.

Paper ID: 193

Experimental study on combustion and NO characteristics of ammonia-hydrogen mixture in lab-scale flameless combustion system

Jiho Yu (Yonsei University / KITECH), Jinje Park (Korea Institute of Industrial Technology), Jongsup Hong (Yonsei University), Youngjae Lee (Korea Institute of Industrial Technology)

The world is consistently looking for various business models in all industries for 2050 carbon neutrality. As a carbon-free fuel, hydrogen is attracting attention in many industries and ammonia is emerging as a hydrogen storage medium. Unlike methane, it contains nitrogen in its molecular structure, so it is necessary to consider nitrogen oxides that can be additionally formed as the fuel-NOx. This study was conducted to analyze the characteristics of flameless combustion and NO emissions using NH_3-H_2 mixtures in the lab-scale flameless combustion system. Thermal NO was reduced by decreasing the peak temperature through flameless combustion. Fuel NO produced by the NH_3 oxidation was reduced by various operating parameters such as the excess O_2, the ammonia supply strategy, and the mixing rate of reactants. Through this study, it was found that the ammonia supply strategy and the control of equivalence ratio are important parameters to control NO formation.

Paper ID: 195

A unified definition of the mixture fraction in nonpremixed ammonia-hydrogen flames

Lorenzo Angelilli (KAUST), Pietro Paolo Ciottoli (DIMA), Francisco Hernandez-Perez (KAUST), Mauro Valorani (DIMA), Hong G Im (KAUST)

For nonpremixed combustion, the mixture fraction variables are widely used as a conserved scalar to map out the flame structure in a unified manner. For ammonia-hydrogen flames, however, a proper definition of the mixture fraction variable is difficult due to the presence of fuel-bound nitrogen in ammonia. This work proposes a new mathematical definition of mixture fraction variable as a modified form of the Bilger's formula in order to describe the characteristics of nonpremixed ammonia-hydrogen blend flames at general fuel mixture ratios. The newly defined mixture fraction properly accounts for differential diffusion effects in the presence of hydrogen, and thus serves as a convenient invariant coordinate for the flame manifolds. Counterflow nonpremixed flames with different ammonia-hydrogen ratios were computed and the validity of the new formulation is demonstrated. Finally, the participation indices obtained through the computational singular perturbation analysis reveal the role of oxidation/pyrolysis of ammonia in the rich side of the flame.

Paper ID: 196

Spray and flow field characterizations of a two-stage counter-swirl injector

Tao Chen (Shanghai Jiao Tong University), Liangliang Xu (Shanghai Jiao Tong university), Bowen Yu (Shanghai Jiao Tong University), Xiaoxing Feng (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University), Xi Xia (Shanghai Jiao Tong University)

This paper presents an experimental study on the spray characteristics and flow structures of a two-stage counter-swirl injector. Three main spray patterns are detected, namely, conical spray, circular spray, and swirling jet spray. The time-resolved spray flow field is obtained using a 10 kHz particle image velocimetry (PIV) system. Based on the analysis of spray morphology and flow field, the spray angle increases rapidly with the air flow rate for the conical spray but tends to saturate for the circular spray. The flow field changes dramatically when the air flow rate increases from 900 to 1300 lpm, showing a strong swirling flow with a large-scale central recirculation zone (CRZ); meanwhile, the spay extends out radially and yields a denser droplet concentration. When the air flow rate increases to 2100 lpm, a swirling jet emerges with disappearing CRZ and high-frequency periodic motions. Furthermore, the size of the CRZ for the circular spray is further quantified based on the circulation of the inner shear layer, showing a strong dependence of the spray performance on the swirling flow field.

Paper ID: 197

Experimental research on turbulent flame propagation of solid particle cloud–gaseous fuel two-phase hybrid mixture co-combustion

Yu Xia (Tohoku University), SeungMin Song (Hokkaido University), Nozomu Hashimoto (Hokkaido University), Osamu Fujita (Hokkaido University)

A two–phase hybrid mixture of solid particle cloud–combustible-gas can be found in many applications/industries, such as low emission thermal power generation (pulverized coal and ammonia) and general manufacturing (dust and volatiles). Understanding turbulent flame propagation of two-phase hybrid mixture co-combustion is essential for achieving a carbon-neutral and safety production society. In two-phase hybrid mixture co-combustion, the interaction between solid particle combustion and gaseous fuel combustion plays an essential role in the turbulent flame propagation phenomena. In present research, to understand the effect of gaseous fuel combustion on turbulent flame propagation of co-combustion, experiments were conducted by varying the turbulent flame speed of gaseous fuel combustion and gaseous fuel types. The consistency of the results between the current study of PMMA particle cloud–methane co-combustion and the previous study for particle cloud–ammonia co-combustion (Xia et al., 2021, 2022 [1,2]) was obtained. The results showed that, in co-combustion, two main effects induced by the particles affect the turbulent flame propagation of gaseous fuel combustion, including the local equivalence ratio increment effect by the addition of volatile matter released from the particles and the negative effect of the heat sink by the unburned particles in the preheat zone of the flame front. Further, in co-combustion, with the increase in the turbulent flame speed of gaseous fuel combustion, the overall effect induced by the reactive particle on the turbulent flame propagation of premixed gaseous-fuel–oxidizer shrinks. On the other hand, the effect was enhanced by reducing the particle size. In co-combustion, the particle devolatilization behavior and chemical reaction of volatile matter–gaseous fuel dominate the turbulent flame propagation phenomena.

Paper ID: 198

Experimental study on operating conditions for NO reduction in lab-scale H_2 flameless combustion system

Eunji Lee (KITECH / UST), Jinje Park (Korea Institute of Industrial Technology), Jiho Yu (Yonsei University / KITECH), Sojeong An (Yonsei University), Won Yang (Korea Institute of Industrial Technology), Youngjae Lee (Korea Institute of Industrial Technology)

With the goal of becoming carbon neutral by 2050, many efforts are being made worldwide to reduce the use of hydrocarbon-based fuels. It is possible that there will be a demand for heat and energy production through the combustion of hydrogen as a carbon-free fuel. However, the application of hydrogen in the combustion field requires technologies that can solve the problems of the control of fast flame speed, high adiabatic flame temperature, and high NOx generation. In this study, NOx generated from hydrogen combustion was experimentally suppressed through flameless combustion, and the performance evaluation was performed for various operation parameters (fuel velocity, dilution, and equivalence ratio) to further reduce NOx. Through this study, the control factors that can minimize NO formation when hydrogen is used as a fuel in combustion devices were derived.

Paper ID: 199

Revisiting the ignition and combustion processes of iso-octane droplet

Hengyi Zhou (Tsinghua University), Haiyu Song (Tsinghua University), Wenyi Zhang (Tsinghua University), Wenkai Liang (Tsinghua University), Yu Cheng Liu (Tsinghua University)

In many experimental studies of iso-octane droplet burning in air, there has been no solid evidence for self-sustaining cool flame or two-stage ignition. However, recent development of chemical kinetics of iso-octane has suggested that multi-staged low temperature combustion (LTC) can take place under certain conditions. Whether the LTC can be demonstrated in a droplet burning configuration, and why it has not been well demonstrated motivated the present study. The numerical simulation for a constant pressure reactor was used to demonstrate various combustion modes due to the isomeric effects in the LTC. Ignition processes of single iso-octane droplets under various conditions were then numerically investigated. A hot ignition case was analyzed in detail. In that case, three heat release rate peaks were found along the radial direction in the gas phase across a large temperature gradient. More evidences of stable cool flame or the first stage ignition will be observed in the following studies.

Paper ID: 200

The impact of Soret diffusion on the product gas characteristics of premixed laminar ammonia/hydrogen/air flames stabilised in a stagnation flow

Marina Kovaleva (Cardiff University), Gabriel J Gotama (The University of Melbourne), Akihiro Hayakawa (Tohoku University), Ekenechukwu Okafor (Kyushu University), Sophie Colson (Tohoku University), Andrew Crayford (Cardiff University), Taku Kudo (Tohoku University), Hideaki Kobayashi (Tohoku University)

Accurate prediction of ammonia/hydrogen flame emissions is important towards an efficient low-carbon energy future and requires accurate modelling of molecular diffusion to account for hydrogen's high diffusivity. The present work investigates the contribution of the Soret effect to molecular diffusion in a laminar burner-

stabilised stagnation flame configuration using a blend of ammonia/hydrogen/air. Addition of the Soret effect in the diffusion model changes the predicted emissions of NO, increases the prediction of NO_2, and reduces N_2O and H_2 predictions. Diffusion flux analysis shows that the Soret effect acting directly on the molecule is predominantly responsible for changes in NO_2 and H_2 profiles. However, NO and N_2O emissions were indirectly affected by Soret diffusion through a change in rates of reaction involving these molecules. In the lean condition, the Soret effect drives enrichment in the flame zone through promoting H_2 diffusion towards the flame front and shifting the flame upstream. In the rich condition, enrichment of the post-flame zone through enhanced NH_3 and H_2 diffusion increases reaction rates of NO and shifts the flame downstream. Therefore, this study informs the underlying behaviours of the Soret effect in influencing ammonia/hydrogen flame chemistry.

Paper ID: 201

A temporally-resolved energy deposition behavior analysis on the creation of laser-induced plasmas in combustion environments

Shu Chai (Shanghai Jiao Tong University), Haimeng Peng (Shanghai Jiao Tong University), Wendong Wu (Shanghai Jiao Tong University)

Energy deposition behaviors are critical to the successful implementations of techniques based on laser-induced plasmas (LIP) in combustion fields. This work studied the energy deposition behaviors of LIP in combustion environments using a temporally resolved approach. With a nanosecond laser operating at multiple longitudinal modes, the breakdown initiation moment was determined with 0.1 ns resolution, by matching the random temporal features of incident and transmitted laser pulses shot-to-shot. We defined the duration from the breakdown initiation moment to the ending time of incident pulse as the post-breakdown region. As the gas temperature increased, the delayed breakdown initiation moment combined with the reduced averaged energy deposition efficiency in the post-breakdown region resulted in the decreased total deposited energy. Furthermore, under an incident energy level of 80 mJ, the relative contributions by the fluctuations of breakdown initiation moment and averaged energy deposition efficiency in the post-breakdown region to the total fluctuations of deposited energy were comparable. This work will promote a deeper understanding on the energy deposition process of LIP in combustion environments.

Paper ID: 202

Experimental investigation of burned gas distribution in high temperature air combustion fueled by NH_3-CH_4 in a bench scale furnace

Apurba Sharma (Hiroshima University), Yimin Qiao (Hiroshima University), Yuji Wakata (Hiroshima University), Yuki Hayashi (Hiroshima University), Tomohisa Miyake (Sanken Sangyo CO.,LTD), Tsukasa Kishimura (Sanken Sangyo CO.,LTD), Takahisa Sonoda (Sanken Sangyo CO.,LTD), Akira Miyoshi (Hiroshima University), Daisuke Shimokuri (Hiroshima University)

Ammonia is one of the most important fuels to achieve a carbon-free society. But, the NO_x emission, which is a major drawback for ammonia combustion, needs to be efficiently controlled. The target of this research is to apply ammonia to metal heating furnaces in which high temperature preheated air (over 1300 K) is utilized. Then, in this study, a bench-scale furnace that can realize a high temperature air combustion field has been

developed. At first, 30% ammonia and 70% of methane based on the lower heating value (LHV) are used as fuel. The appearance of the combustion field, exhaust gas composition, and gaseous distributions inside the furnace have been investigated for an equivalence ratio of 0.9 and the thermal input of 40 kW. Result shows that the intensity of chemiluminescence of NH, CN and OH radicals is significant, and NOx emission is quite high for the high temperature air combustion. The results of gaseous measurements inside the furnace revealed that the NO concentration inside the furnace is quite high at all measured points, which suggests that the NH_3 is converted into NO rapidly and efficiently inside the furnace.

Paper ID: 203

Multi-fidelity neural network-based surrogate model for uncertainty quantification of combustion kinetic models

Chengcheng Liu (Tsinghua University), Keli Lin (Tsinghua University), Yiru Wang (Tsinghua University), Bin Yang (Tsinghua University)

Uncertainty quantification (UQ) is essential to improve the confidence level of chemical reaction kinetic models with parameter uncertainties. The artificial neural network-based surrogate model could efficiently generate model prediction samples for UQ tasks. However, the generation cost of training samples under multiple operating conditions is high for large hydrocarbon fuels. In the present work, we propose a multi-fidelity neural network-based surrogate model (MFNNSM) to alleviate this problem. The MFNNSM contains two separate neural networks. The first neural network learns the correlation between model predictions, then generates samples to train the second neural network for the subsequent UQ analysis. This method is tested on methanol and n-decane ignition systems. The results show that the acceleration ratios in the methanol and n-decane systems under the same ignition condition are 1.17 and 2.67, respectively. Moreover, the MFNNSM has realized the acceleration factor of 2 and 5 by reusing the reduced model predictions from different ignition conditions. The proposed method provides a new perspective for reducing the cost of UQ analysis for large chemical reaction models.

Paper ID: 204

Machine learning-based prediction of global equivalence ratio from absorption spectra on a swirl combustor

Cheolwoo Bong (Sungkyunkwan University), Moon Soo Bak (Sungkyunkwan University), Yongjun Kwon (Sungkyunkwan University)

A new optical scheme that predicts a global fuel-air equivalence ratio of a swirl combustor from a limited set of absorption spectra is proposed in this study. Once the combustor is under normal operation, the temperature and concentration fields are determined by global equivalence ratio and total flow rate. Therefore, changes in absorption spectra of water vapor at wavelength ranges around 1343.34, 1391.6, and 1469.3 nm measured at three different downstream locations of the combustor were mapped to the global equivalence ratio, and since it is difficult to find analytical relationships between these values, a predictive model was acquired data-drivenly. the absorption spectra as an input were first feature-extracted through convolutional autoencoders (CAEs) and then a dense neural network (DNN) was used for regression prediction between the feature scores and the global equivalence ratio. The model was found to predict the equivalence ratio with an absolute error

of +- 0.025 with a probability of 96 %.

Paper ID: 205

Rapid flame acceleration and deflagration-to-detonation transition in flowing mixtures

Wandong Zhao (National University of Defense Technology), Xinxin Wang (National University of Defense Technology), Jianhan Liang (National University of Defense Technology), Xiaodong Cai (National University of Defense Technology), Ralf Deiterding (University of Southampton)

An unconventional method of flame acceleration propagating upstream in subsonic and supersonic mixtures is proposed to obtain a rapid onset of detonation. The Navier-Stokes equations with adaptive mesh refinement and a detailed hydrogen-air chemistry reaction mechanism of 11 species and 27 steps are employed to simulate the whole flame propagation and the deflagration-to-detonation transition (DDT) characteristics. The effect of the initial Mach number on flame acceleration and the DDT mechanism are discussed in detail. It is found that a rapid oblique shock wave occurs when flame propagates upstream along the upper and lower walls due to the boundary layer influence. An intense coupling between the shock and the leading flame tip is enhanced by increasing the initial Mach number of the mixture. Hence, the run-up DDT time is shortened accordingly through the direct detonation initiation as a result of the strong leading shock wave after it reflects from the right side of the confined wall. The prompt formation of the oblique shock wave is formed at the incipient stage, mainly caused by the boundary layer influence and the coalescences of the compressive waves.

Paper ID: 206

Experimental and modeling study of ignition delay times of natural gas mixtures with CO_2 dilution

Wenxiang Xia (Huazhong University of Science and Technology), Jinling Yang (Guangdong Midea Kitchen& Water Heater Appliances Manufacturing Co.Ltd), Chun Zou (Huazhong University of Science and Technology)

Pressurized oxy-fuel combustion has gained great concern owing to its low emission and high efficiency. Natural gas is a clean fossil fuel and is widely utilized for combustion applications including gas turbines, which can be appropriately represented by a $CH_4/C_2H_6/C_3H_8$ mixture. In this study, the ignition delay times of 90%CH_4/9%C_2H_6/1%C_3H_8 mixture diluted in CO_2 were measured at pressures of 2 and 10 atm; equivalence ratios of 0.5, 1.0, and 2.0; and temperatures in the range of 1280-1645 K in a shock tube. Several key reactions in the OXYMECH 2.0 model were updated and the modified model named OXY-NG shows reasonable performance in the prediction of ignition delay times in both O_2/N_2 and O_2/CO_2 atmospheres. Two artificial species are introduced to quantitively analyze the effects of the physical and chemical properties of CO_2 at different conditions in detail.

Paper ID: 207

Shock tube and modeling study of ethylene and propene ignition delay times diluted in O_2/CO_2 atmosphere

Chao Peng (Huazhong University of Science and Technology), Chun Zou (Huazhong University of Science and Technology)

Pressurized Oxy-fuel combustion of fossil fuels have attracted attention of researchers due to high power cycle

efficiency with the carbon capture. Olefin molecules are important intermediates in the oxidation of macromolecular hydrocarbons. In this work, the ignition delay times of ethylene and propene diluted in CO_2 were measured at the pressures of 1 and 10 atm at three different equivalence ratios (0.5, 1.0, 2.0) in a shock tube, respectively. A detailed model was updated based on our previous work and validated by the experimental data. The present model well reproduced the combustion characteristics of ethylene and propene from both our experiments and data from literatures. The present model was compared with NUIGMECH1.1 model for the prediction of ignition delay times in CO_2 atmospheres and laminal flame speeds in detail.

Paper ID: 208

A study on diagnosis of combustion instability using various statistical analysis of dynamic pressure signals

Dae Jin Jang (Incheon National University), Min Kuk Kim (Korea Institute of Machinery and Materials), Jeongjae Hwang (Korea Institute of Machinery and Materials), Min Chul Lee (Incheon National University)

Recently, decarbonized fuels such as hydrogen and ammonia are attracting attention due to the de-carbonization issue of power plants. Since these fuels have different combustion characteristics from conventional fossil fuels, more sophisticated combustion instability diagnosis is required to operate the combustion system safely and stably. A diagnosis of combustion instability is studied by using various statistical analyses, such as permutation entropy, energy of entropy, zero-crossing rate, spectral spread, and filter bank. The performance of each concept is validated by dynamic pressure data obtained from a gas turbine combustion experiment. Based on data measured in a partially premixed nozzle burner, six types of combustion instability criteria in dynamic pressure were compared. An early detection of combustion instability was possible by applying the zero-crossing rate method. As a result, it was 0.42 seconds faster than conventional root mean square method. The results of this study could be applied to a detection and control system of gas turbine combustors.

Paper ID: 209

Experimental and modelling investigations of methanol fuels with different fractions of ignition additives in a compression-ignition engine

Chong Cheng (DTU), Rasmus Faurskov Cordtz (DTU), Jesper Schramm (DTU)

In order to investigate the combustion process of methanol fuel on an engine and to simulate the process in a model, experimental and simulation investigations were carried out on a compression-ignition (CI) Bukh engine using methanol with ignition additive. First, the experimental heat release rate (HRR) of the engine was measured, followed by a simulation of the HRR using a multi-packet model and a comparison of the experimental and simulated HRR. Intermediate simulation variables (including velocities, air masses, droplet evaporation, air/fuel equivalence ratios, burning packet temperatures in different packets) were also analyzed in detail. These variables are essential for the simulation of the methanol combustion process and the subsequent modelling of emission pollutants. For methanol fuels with 5% and 7.5% ignition additives, the combustion process was analyzed as a partially premixed combustion (PPC) process. The ignition delays were 1.38 ms and 0.94 ms, respectively.

Paper ID: 210

Numerical investigation of the detonation initiation in a model rotating detonation engine

Chao Han (Beijing Institute of Technology), Cheng Tian (Beijing Institute of Technology), Majie Zhao (Beijing Institute of Technology)

In experiments, the one-way pre-detonator is widely used to ignite rotating detonation engines, while sometimes two-way detonation waves are formed in the combustion chamber. In order to further study the mechanism behind this phenomenon, in this study, high resolution two-dimensional numerical simulations are conducted to investigate the influence of the channel width on the detonation initiation and the detonation propagation characteristics in stoichiometric hydrogen-air mixtures in rotating detonation engines. The results show that two-way detonation waves are more likely to form when increasing the channel width. It is mainly because that the height of premixed gas near the combustion chamber inner wall increases with the increase of the channel width. In addition, it is found that the speeds of detonation waves propagating clockwise is roughly equal to that of detonation waves propagating counterclockwise.

Paper ID: 212

Parametric analysis on ignition assistance by a shielded hot surface under aircraft compression ignition engine conditions

Sayop Kim (New York University Abu Dhabi), Je Ir Ryu (New York University Abu Dhabi), Austen Motily (University of Illinois Urbana-Champaign), Tonghun Lee (University of Illinois Urbana-Champaign), Kenneth S Kim (US Army Research Laboratory), Chol-Bum M Kweon (US Army Research Laboratory)

This study describes optimized ignition assistance (IA) strategy regarding the parametric factors of IA devices, which supports ignition control, for aircraft compression ignition engines. Such an ignition control technique can effectively support reliable engine operation against varying altitude conditions by means of active ignition timing control. The ignition performance may vary as a function of the IA device's thermal impact and geometrical configuration and often be limited by the complex nature of the thermo-chemical process in the combustion chamber. Therefore, ultimate CI engines may require optimization of such design parameters. To this end, this study examines various parametric elements by implementing the design of experiments (DoE) analysis. The IA device with an obliquely 45-degree cut shield was used to assess the geometrical impact, and the impact of IA device temperature was added for the analysis. Total 37 numerical experiment cases were chosen for DoE input factors. The DoE analysis constructed a regression equation to express the predictive response function, which was then utilized to provide insights into ignition enhancement performance against the reference cases with bare IA devices without the shield design.

Paper ID: 213

The role of gas supply-driven instability on dynamic flame responses and combustion instability

Jaehyun Nam (Seoul National University), Jack J. Yoh (Seoul National Univ Korea)

In this study, large eddy simulations (LES) of the model gas turbine combustors are performed to investigate the cause of the flame and flow responses inside a combustor. Partially premixed turbulent flame is considered and the external acoustic forcing function in the frequency range of 0-600 Hz is given at the combustor inlet. In the simulation results, it is found that the flame responses are strong only at certain forcing frequencies,

resulting in a high gain of the flame transfer function (FTF). It is noticed that turbulence and acoustics inside a fuel supply line predominantly affect the flow responses in the combustor, resulting in high gain in FTF characteristics. The obtained FTF data is validated with the experimental results, and a good agreement is seen between the simulated and experimental results. The thermoacoustic instabilities inside the combustor are subsequently simulated, and the relation between fuel-air mixing in the swirler and the triggered instability is investigated. The results confirm that the frequencies of equivalence ratio fluctuation coincide with pressure instability frequencies. Therefore, it is concluded that incomplete mixing at the nozzle affects the combustion instabilities inside a combustor.

Paper ID: 214

Theoretical study of proton transfer reaction in energetic ionic compounds

Jay Patel (Indian Institute of Technology Bombay), Arindrajit Chowdhury (Indian Institute of Technology Bombay), Neeraj R Kumbhakarna (Indian Institute of Technology Bombay)

The objective of this work is to gain a better understanding of the condensed phase initiation reaction involving proton transfer in ionic energetic materials such Guanidinium azotetrazolate, triaminoguanidinium azotetrazolate, guanidinium nitrate, ammonium nitrate and ammonium perchlorate. When investigating chemical reactions that include protonation and deprotonation, it is essential to know the proton affinities (PA) of the species that are involved. High-level quantum chemical computation method, CBS-QB3 was used in this work to estimate the proton affinity for the cations and anions in the condensed phase. The calculations show that proton affinitues of all cations are quite high as compared to those of the relevant anions; as a result, a direct proton transfer reaction does not take place in the condensed phase. It may of may not take place in the gas phase because even though the PA values favour it, structural orientation of the ionic species might not be conducive.

Paper ID: 221

Effect of fire position on fire phenomena in two rooms connected through vertical opening

Yun Young Kim (Pukyong National University), Chi Young Lee (Pukyong National University)

The effect of fire position on the fire phenomena in two rooms (i.e., ROOM1 and ROOM2) connected through the vertical opening was numerically investigated under various heat release rate conditions. ROOM1 indicates the room with a single opening connected to ROOM2. ROOM2 indicates the room with two openings connected to ROOM1 and outside. When fire occurs in ROOM1 and ROOM2, which indicates ROOM1_F and ROOM2_F, respectively, the flow velocity distribution and mass flow rate through the vertical openings were examined. In addition, for the fire room and its adjacent room of ROOM1_F and ROOM2_F, the temperature distribution, hot gas layer thickness, and hot gas layer temperature were reported and discussed. The velocity distributions through the vertical openings for ROOM2_F were different from those for ROOM1_F. Fire room for ROOM1_F showed higher temperature distribution, thicker hot gas layer, and higher hot gas layer temperature than that for ROOM2_F. Adjacent room for ROOM1_F exhibited higher temperature distribution, thinner hot gas layer, and higher hot gas layer temperature than that for ROOM2_F. These trends were closely related with the mass flow rate results.

Paper ID: 222

Mild combustion of a premixed NH_3 jet flame in hot coflow

Guochang Wang (Huazhong University of Science and Technology), Xiangtao Liu (Peking University), Pengfei Li (Huazhong University of Science and Technology), Zhaohui Liu (Huazhong University of Science and Technology), Jianchun Mi (Peking University)

Ammonia (NH_3) is a hydrogen-enriched carbon-free fuel. However, its traditional combustion is hard and produces extremely high NO_x emissions. As a new technology, MILD combustion is very suitable for the fuel of ammonia which burns stably with low NO_x emission. However, the related studies are very rare. This paper reports a numerical study on the combustion and emission features of a premixed NH_3/air jet flame in hot coflow. For comparison, similar CH_4/air JHC flames are also calculated. All the ammonia and methane flames are under MILD regime. Results show that the NH_3 flame has lower temperature rise and larger reaction zone compared to the CH_4 case. The lift-off height is also larger for the NH_3 flame at the equivalence ratio $\phi_J < 1$. However, at $\phi_J > 1$, the lift-off height of the NH_3 flame is lower than that of the CH_4 flame. Moreover, the NO_x emission from the NH_3 flame is much higher than from the CH_4 flame. The NO_x emission from the NH_3 flame is high at $\phi_J < 1$ and quickly drops to near zero at $\phi_J > 1$. However, the emissions of unburned NH_3 and H2 greatly increase. So, the balance of the two factors results in the optimized ϕ_J being about 1.0. In addition, the NO_x emission from the NH_3 flame can be greatly reduced by one to two orders under the MILD regime against the conventional combustion.

Paper ID: 223

Mild combustion characteristics of a premixed ammonia jet flame in hot coflow: effects of coflow temperature and oxygen-level

Guochang Wang (Huazhong University of Science and Technology), Xiangtao Liu (Peking University), Pengfei Li (Huazhong University of Science and Technology), Zhaohui Liu (Huazhong University of Science and Technology), Jianchun Mi (Peking University)

Ammonia (NH_3) is a hydrogen-enriched carbon-free fuel. However, it is troublesome to be burnt conventionally: i.e., hard ignition, unstable combustion and extremely high NO_x emission. Such issues may be solved by using the MILD combustion, a technology newly developed for fossil fuels but barely explored for ammonia. This numerical study is designated to fill the gap by investigating the MILD combustion characteristics of a premixed ammonia Jet-in-Hot-Coflow (JHC) flame versus the methane JHC flame. The specific aim is to examine the effects of coflow temperature (T_C) and oxygen-concentration ($X_{O2,C}$). It is demonstrated that the NH_3 flame generally exhibits lower temperature rise (ΔT), larger reaction zone volume (V_{RZ}) and higher lift-off (H/d) when comparing the CH_4 flame. As T_C rises, ΔT firstly increases and then decreases for both flames but V_{RZ} changes oppositely. H/d drops with T_C and finally both flames attach to the burner exit (H/d = 0) at TC ≥ 1500 K. Moreover, taking T_C = 1500 K, the increase of $X_{O2,C}$ results in higher ΔT and smaller V_{RZ} for both flames and always $H/d \approx 0$. Important, under any conditions, the NH_3 flame produces the NO_x emission (E_{NOx}) that is two orders higher than the CH_4 flame. As T_C rises, E_{NOx} from the NH_3 flame gradually increases and then plateaus at T_C >1500 K. As $X_{O2,C}$ rises, E_{NOx} quickly increases. The optimal coflow condition for low E_{NOx} and stable NH_3 combustion is high T_C (> 1500 K) and low $X_{O2,C}$ (≤ 3%).

Paper ID: 224

Blow-off characteristics evaluations by steady-state rans simulation and transient quasi-dns for a partially-premixed coaxial burner

Kazuki Abe (Tohoku University), Youhi Morii (Tohoku University), Kaoru Maruta (Tohoku University / Far Eastern Federal University)

Steady-state and transient calculations were performed to consider the effect of non-stationarity on flame blow-off characteristics. One burner with a mixing tube downstream of a coaxial jet of fuel and air was considered. The steady-state calculations are performed in RANS using the standard k-epsilon model, and the transient calculations are performed in the DNS manner whose results are guaranteed by mesh convergence, which is called quasi-DNS. Under stable conditions, the RANS calculations produced results with a certain degree of accuracy. However, for flame blow-off conditions, the RANS calculation overestimates the stability compared to the quasi-DNS calculation. It is important to consider non-stationarity in order to obtain accurate results, especially for the flame blow-off condition.

Paper ID: 225

NOx and CO Emissions in a two-stage model gas turbine combustor with a blended fuel of methane and ammonia

Juhan Kim (Ulsan National Institute of Science and Technology), Jeong Park (Pukyong National University), Suk Ho Chung (King Abdullah University of Science and Technology), Chun Sang Yoo (Olsan National University)

The characteristics of NO_x and CO emissions in a two-stage model gas turbine with a blended fuel of methane and ammonia were investigated by varying the bulk flow velocity and equivalence ratio (ϕ_{pri}) in the primary zone. For two-stage combustion, 20% ammonia and 80% methane in volume were used in the primary zone, while air or methane/air was supplied to the secondary zone. The equivalence ratio for methane/air mixture and flow velocity in the secondary zone are fixed to 0.8 and 3 m/s, respectively. For the baseline case, the single-stage premixed flames with methane and ammonia are classified into five regimes: brush flame, M-shape flame, conical flame, columnar flame, and yellow flame around the main flame. CO emission in the single-staged combustion with a blended fuel of 80% CH_4 and 20% NH_3 increased drastically at $\phi_{pri} \geq 1.0$. The similar trend was observed in the two-staged combustion with methane/air injection in the secondary zone. While for air injection in the secondary zone, CO emission increased drastically at $\phi_{pri} > 1.3$. For two-staged combustion, air and methane/air injection in the secondary zone rather decreased NO emission, as compared with those for single-staged combustion. For two-staged combustion, reduction of NO emission with the CH_4/air injection in the secondary zone is more effective than that with pure air.

Paper ID: 226

A hybrid FPV-FRC combustion model based on adaptive scalar transport

Zhiwei Zhao (Shanghai Jiao Tong University), Tongtong Yan (Shanghai Jiao Tong University), Dezhi Zhou (Shanghai Jiao Tong University)

This work details an adaptive scalar transport (AST) framework dynamically dividing scalar quantities of combustion field into groups, which are either solved by transport equations or mapped from lower-order

manifolds. The idea generated here is to utilize low manifold topology model's merits as bypassing the species transport as well as temporal integration of chemical source terms, and meanwhile maintain adequate predictive accuracy through detailed chemistry computation for chemically slow species, which often have poor correspondence in the topology-based strategy. The species dividing criterion is constructed based on a drift error examination between detailed transportation and mapped results from low-order manifolds. To validate AST, corresponding simulations are conducted on a laminar, multi-modal triple flame with Finite Rate Chemistry (FRC) and Flamelet Progress Variable (FPV) as two sub-models of the hybrid framework. From the results, AST's computational cost is noticeably reduced compared with FRC as fewer species are transported and scalars like diffusivities can be directly mapped, while the fidelity is significantly improved from FPV especially for scalars with strong FRC effects. The developed AST framework provides a multi-modal combustion modeling framework to achieve both accurate and efficient reacting flow simulations and is very promising to extend to turbulent combustion modeling.

Paper ID: 227

Peculiar characteristics of magnesium subjected to hygrothermal aging

Yejun Lee (Seoul National University), Juyoung Oh (Seoul National Univ Korea), Jack J. Yoh (Seoul National Univ Korea)

Magnesium is emerging as a good alternative to fossil fuels in that it can generate a lot of heat energy without CO_2 emission. While increasing the use of magnesium, the deterioration of magnesium performance by aging has not been identified clearly. An oxide film, which is composed of magnesium oxide (MgO) and magnesium hydroxide ($Mg(OH)_2$), is formed during hygrothermal aging. MgO tends to desensitize the magnesium oxidation, whereas $Mg(OH)_2$ accelerates the reaction. Since magnesium oxide is predominant in oxide film, magnesium oxide film makes the reaction desensitize. In addition, after 25 weeks of aging period, only core oxidation occurred due to the formation of a sufficient oxide film. Thus, this study clarifies that magnesium subjected to hygrothermal aging has some peculiar changes of reactivity and how oxide film affects magnesium oxidation.

Paper ID: 228

A study on thermal decomposition of N_2O in high temperature reactor

Suhyeon Kim (Korea Maritime&Ocean University), Sung Hwan Yoon (Korea Maritime & Ocean University), Seung-Gon Kim (Korea Institute of Energy Research), Daegeun Park (Korea Institute of Industrial Technology)

As global interest in global warming grows, each country has set goals to reduce greenhouse gas emissions. N_2O has a high Global Warming Potential (GWP) and depletes the ozone layer with a stable structure. In this experiment, a high-temperature electric furnace was adopted as the experimental equipment, and experimental results and numerical results were compared and analyzed. As a result, the N_2O decomposition rate increased as the reaction temperature increased, and most of the decomposed N_2O was converted to N_2. Almost of N_2O were decomposed at the reaction temperature of 1500 K in both experiment and numerical result.

Paper ID: 229

An experimental study on thermal runaway of lithium-ion battery by external temperature

Juwon Park (Korea Maritime & Ocean University), Sung Hwan Yoon (Korea Maritime & Ocean University)

The purpose of this study is to experimentally observe the mechanism for the thermal runaway of a lithium-ion battery and propose a technology to suppress the thermal runaway. Thermal runaway of the lithium-ion battery was observed by adjusting the supplied heat transfer coefficient and SOC level, and an inert gas was formed in a chamber to suppress the thermal runaway. As a result, if the internal temperature of the lithium-ion battery increased, it was determined that a thermal runaway caused by the internal defect of the lithium-ion battery would in-evitably occur. The lithium-ion battery consists of cathode material, anode material, separator, and electrolyte, but if the structure of the separator is damaged due to internal or external defects, the chemical reaction caused by the short circuit between the cathode material and anode material causes a thermal runaway. However, it is observed that thermal runaway is suppressed because of the reduction of internal energy if the SOC-level is below 80% in this study, through this study, we will discuss how to quickly extinguish a fire caused by thermal runaway even if thermal runaway occurs.

Paper ID: 230

A quasi-continuous description of activity coefficients applicable for preferential vaporization of complex liquid fuels

Yuhang Sun (Tsinghua University), Yu Cheng Liu (Tsinghua University)

Complex liquid fuels naturally contain hundreds of species with different volatility and preferential vaporization can further complicate modelling of droplet vaporization simulations. Modelling deviation from ideal mixture (represented by activity coefficients in this work) can be very challenging for continuous models due to their complicated correlations dynamically associated with all the components. A quasi-continuous model (QCM) of activity coefficient applicable for vaporization of complex liquid fuels was introduced in this work. Similarity of the same hydrocarbon family in UNIFAC method was assumed to facilitate transforming description of activity coefficients and diffusion coefficients into a continuous form. To validate the efficacy of QCM, the results of distillation simulation for a complex liquid fuel (Chinese jet fuel RP-3) were compared with those with a detailed discrete model of 40 components (DCM) as the target. Results with QCM demonstrated great predictability on activity coefficients and diffusion coefficients, so that distillation curve, variation of groups fraction and properties in liquid and gas phase during distillation can be well captured. QCM for the distillation simulation demonstrated in this study can save about 90% of CPU time comparing to DCM.

Paper ID: 231

The effects of diluents addition on the OH and PAH formation in inverse-coflow laminar diffusion flames

Raul A. Serrano Bayona (King Abdullah University of Science and Technology), Peng Liu (King Abdullah University of Science and Technology), Et-touhami Es-sebbar (King Abdullah University of Science and Technology), William Roberts (KAUST)

The inverse coflow diffusion flame (IDF) is the basis in the autothermal reforming of natural gas. However,

the formation of polycyclic aromatic hydrocarbons (PAH) and soot is unavoidable for high-pressure IDF. This study assesses the effects of various diluents including carbon dioxide (CO_2), nitrogen (N_2), argon (Ar), and helium (He) in the fuel stream over the formation of OH radicals and PAHs in IDF. The planar laser-induced fluorescence was applied to obtain the OH and PAH information. Results show that adding diluents decreases the PAH signal and increases the height of the OH region, with the highest influence exerted by the CO_2. The peak OH intensity remains nearly constant for all CO_2, N_2, and Ar flow rates. However, using He slightly reduces the OH signal, which can be associated with a decrease in the flame temperature. The provided experimental data could serve as model validation.

Paper ID: 232

Experimental spray characterization for jet-a1 under temperature controlled subcritical, transcritical, and supercritical spray conditions

Kaushik Nonavinakere Vinod (North Carolina State University), Robert Kempin (NC State University), Tiegang Fang (NC State University)

Fuels when sprayed under superheated and elevated fuel pressure show different behavior than traditional fuel injection sprays. In this work optical diagnostics were used to study the behavior of Jet A-1 under subcritical, transcritical, and supercritical sprays into open air ambience. Five different temperatures were tested, and the resultant spray images were processed to obtain quantitative measurements such as spray penetrations, and spray cone angle for each case. The spray structure transition with changing parameters from subcritical, transcritical, and supercritical states were also studied. The transition between the three different states are shown in this study and the resulting spray cone angles and penetrations are compared for the fuel. The results show that a transcritical spray has a measurable variation in the spray cone formation and penetration process for a fixed injection pressure. At this state the spray cone shows a bimodal spray angle relationship with increasing penetration. Flash boiling of the fuel is observed near the nozzle of the injector. Increasing the temperature further into the supercritical regime, the spray plume shows a thinning of the jet near the nozzle with a reduced overall penetration compared to lower temperatures.

Paper ID: 234

A study on the vitiation air heater for the direct-connect Scramjet combustor and preliminary ignition test of the Scramjet combustor.

Inhoi Koo (Pusan National University), Jae-Hyuk Lee (Pusan National University), Min-Su Kim (Pusan National University), Eun-Sung Lee (Pusan National University), Hyung-Seok Han (Pusan National University), Jeong-Yeol Choi (Pusan National University)

The combustion characteristics of the vitiation air heater (VAH) for direct-connect scramjet combustor were experimentally studied. The VAH consists of a head, modular chamber, and circular to rectangular shape transition (CRST) nozzle. The CRST nozzle transforms the circular cross-sectioned rocket-type VAH into a rectangular cross-sectioned scramjet combustor. The CRST nozzle exit Mach number at the top, middle, and bottom were measured using a wedge. The oblique shock formed by the wedge was captured by Schlieren visualization and recorded with a high-speed camera. The θ-β-M relation showed that the exit Mach number was 2.04±0.04 at a chamber pressure of 1.685 ± 0.07. With the VAH design point verified, preliminary

scramjet combustor ignition tests were conducted. As the fuel was not auto-ignited by the vitiated air, the forced ignition method, in which VAH ignition flame ignites the scramjet fuel, was used. The Schlieren images showed that a cavity shear layer combustion mode was formed and showed that the forced ignition method could be used as a reference model for the ignitor-ignition method.

Paper ID: 235

An experimental study on the ignition of Scramjet combustor using μPDE

Lee Keon Hyeong (Pusan National University), Jae-Hyuk Lee (Pusan National University), Min-su Kim (Pusan National University), Eun-Sung Lee (Pusan National University), Hyung-Seok Han (Pusan National University), Jeong-Yeol Choi (Pusan National University)

The ignition and combustion characteristics of the scramjet combustor were experimentally studied using a direct-connect scramjet combustor (DCSC). The DCSC provided vitiated air at a total pressure of 1.685±0.07 MPa, a Mach number of 2.04±0.04, corresponding to flight altitude of 20~25 km, and a Mach number of 5.0 to the isolator and scramjet combustor. The wall pressure profile and high-speed Schlieren imaging were used to observe the combustion characteristics according to the equivalence ratio. A micro-pulse detonation engine (μPDE) produced a high-temperature and high-pressure plume. Parametric studies to determine μPDE conditions were conducted: minimum mass flow rate with maximum detonation pressure. The Schlieren images showed that the shock wave created by the detonation wave lingered at the cavity leading edge, leading to a peak pressure of the scramjet combustor. The combustion area was confined in the cavity shear layer at $\phi = 0.04$. The cavity leading edge induced shock wave interacted with the boundary layer, and the circulation zone was formed under the triple point. The pressure profile showed that as the equivalence ratio increased, the upstream cavity pressure increased. The exit pressure of each case was higher than the atmospheric pressure, expected to create the expansion shock at the outlet.

Paper ID: 237

Substitutability of core materials for fire doors

Che-Ming Hsu (National Cheng Kung University)

This study has a collection of 100 fire door reports and is commonly used with core materials which were compiled. There were totally 16 specimens designed all over this study, without considering structural design and hardware accessories. After experimenting and analyzing, it was found that rock wool is just lighter than ceramic wool and has better heat resistance; fiber cement board is as-well heavier than calcium silicate board and gypsum board and has a poorer heat resistance; calcium silicate board is slightly heavier than gypsum board, and their thermal resistance are close. Therefore, it is considerably feasible to replace the ceramic wool with rock wool, or replace fiber cement with calcium silicate board or even on gypsum board. Calcium silicate board and gypsum board can be however interchanged when they have similar properties.

Paper ID: 238

Temperature measurement in laminar flames by oh thermally assisted lif method based on a single broadband femtosecond laser

Sibo Huang (Tokyo Institute of Technology), Mamoru Tanahashi (Tokyo Institute of Technology), Masayasu

Shimura (Tokyo Institute of Technology)

This paper introduces a new two-dimensional temperature measurement method by thermally assisted OH laser-induced fluorescence (TALF) in OH A Σ v' = 0 energy level and tested it in different CH_4/air laminar flames (φ = 0.8, 0.9, 1.0, 1.1, 1.2). In this method, single-photon excitation of OH A $\Sigma \leftarrow$ X Π (0 - 0) is achieved by a single broadband femtosecond laser around 307 nm, and the spatial distributions of the OH fluorescence of (0 - 0) and (1 - 0) bands are captured by two CMOS cameras instantaneously. It is found this method can be effectively applied in the burnt area, where the measured temperature in the range of 1600 - 2000 K is almost linearly to the ratio of the (1 - 0) and (0 - 0) fluorescence. At the same time, OH chemiluminescence and fluorescence quenching with oxygen and nitrogen significantly limit the accuracy in the flame edge area. In conclusion, this method can measure the temperature distribution with high frequency by a simple experiment setup with a single laser source in the hot burnt area.

Paper ID: 239

A numerical study on fire whirls formed behind an L-shaped wall

Ashutosh Bharti (Indian Institute of Technology Madras), S Muthu Kumaran (Worcester Polytechnic Institute), Vasudevan Raghavan (Indian Institute of Technology Madras)

This work presents a numerical study on fire whirls formed behind an L-shaped wall in cross-flow. The simulations have been carried out using Fire Dynamics Simulator (FDS v.6.7.9), an open source numerical tool suitable for simulating low Mach number, thermally-driven flows. The numerical model is validated with the experimental data available in literature. Results show that the fire whirl exist only for a specific range of air velocities characterized by Fire Froude number in the range $0.025 \leq Fr \leq 0.055$. The mass loss rate gradually increases with the cross-flow velocity for the cases with fire whirl and decreases steeply when the whirl ceases to exist. The velocity profiles show strong rotation and air entrainment near the base of the flame. It also depicts the movement of fire whirl closer to the L-shaped wall with systematic increase in cross-flow velocity. The predicted temperature and species concentration profiles show the variation in flame structure within a fire whirl in cross-flow.

Paper ID: 240

Effects of composition on the combustion characteristics of ammonia-hydrogen/air mixtures in a swirl model combustor

Jae Hyun Kim (Sungkyunkwan University), Jae Ho Song (Sungkyunkwan University), Oh Chae Kwon (Sungkyunkwan University)

To demonstrate the practical use of carbon-free ammonia (NH_3)-hydrogen (H_2) blends for responding climate change, the combustion characteristics of NH_3-H_2/air premixed flames in a swirl model combustor are studied. For various conditions of the fuel-equivalence ratio (ϕ) and the mole fraction of H_2 in the fuel blend ($_{xh,f}$), the combustion stability limits and nitrogen oxides (NO_x) emissions of NH_3-H_2/air premixed flames are examined, and their visualization is conducted. Combustion stability limits are broadened with increasing $_{xh,f}$ and mixture injection velocity, due to the high burning intensity of H_2 and the enhanced turbulent effects. The deNO_x effect of NH_3 is observed at fuelrich condition and for pure NH_3 compared with NH_3-H_2 blends. Also, the main reaction zone of the flames shifts to the downstream of the combustor with increasing ϕ and decreasing $_{xh,f}$,

which can be observed from the flame visualization (OH* and NO* chemiluminescence and OH planar laser induced fluorescence). In this study, the database of NH_3-H_2/air premixed flames to utilize NH_3-H_2 blends as a practical fuel is obtained. To consider the thermal cracking of NH_3, a comparative study

on the combustion properties to NH_3-H_2-nitrogen (N_2) and NH_3-H_2 blends under elevated pressure condition is in progress.

Paper ID: 241

Modeling of turbulent flame speed and turbulent Markstein length of a harmonically oscillating flame

Jungho Sohn (Korea Advanced Institute of Science and Technology), Donghyuk Shin (Korea Advanced Institute of Science and Technology)

The modern gas turbine has caused serious environmental problems, such as global warming, climate change, and pollutant emissions due to the usage of carbon-based fuels, and the need for alternative fuels increases. On the circumstance, hydrogen is spotlighted as one of the eco-friendly fuels. However, hydrogen has drastically different combustion characteristics compared to liquid natural gas (LNG), which is the traditional gas turbine fuel, so there is a chance of combustion instability occurrence. To predict and prevent instability, the combustion characteristics, and flame behavior is needed to be investigated. Through the several preceding studies, a simple method of using a reduced-ordered model, i.e. G-equation, has been suggested. In this study, the solution of the G-equation is further investigated using the asymptotic analysis, and the behavior of harmonically oscillating flame is expressed by explicit formulations. Then, the expressions are evaluated using the numerical simulation using the 3D level-set method. The suggested explicit expressions would provide intuition about the combustion characteristics of hydrogen and the effects of turbulence on flame.

Paper ID: 242

Efficiency and cyclic variation of a diesel retrofit using diesel and natural gas

Wan Nurdiyana Wan Mansor (Universiti Malaysia Terengganu), Mohammad Nor Khasbi Jarkoni (Universiti Malaysia Terengganu), Samsuri Abdullah (Universiti Malaysia Terengganu), How-Ran Chao (National Pingtung University of Science and Technology), Sheng-Lun Lin (Beijing Institute of Technology), Daniel B Olsen (Colorado State University)

The development of a cost-effective diesel engine is increasingly challenging for manufacturers due to tightening emission regulations. One of the attractive alternatives for older engines without making significant changes to the engine's design is found to be retrofit techniques to reduce exhaust emissions and increase performance. In this study, a commercial dual fuel system is used to convert a 6.8 liter, 6-cylinder, 4-stroke industrial non-road diesel engine into a dual fuel engine. This research used the ISO Standard 8178:4 Cycle D2 cycle, which consists of five test runs at 1800 rpm. During dual fuel operation, the amount of natural gas injected into the system controls the engine's production of power. Dual fuel thermal efficiency is shown to be lower than diesel operation at low loads, but it improves at mid- and high-load conditions. Thermal efficiency is improved by around 20% at mid and high loads by using natural gas in diesel engines. Brake-specific fuel consumption (BSFC) is influenced by the air/fuel ratio. As the mixture gets leaner, the BSFC increases. At all loads except 100% load, the ignition delays in dual fuel operation are larger. In addition, as compared to the diesel baseline, dual-fuel operations have a longer range and higher variability. To get the full

benefits of the dual fuel engine, the natural gas fed into the engine under lower loads should be switched off. The study findings provide valuable insight for operators to carry out their work on diesel retrofit engines with natural gas.

Paper ID: 243

Effect of inner diameter on horizontal flame spread over electric wire in a cylindrical tube

Anju Funasaki (Hokkaido University), Yusuke Konno (Hokkaido University), Nozomu Hashimoto (Hokkaido University), Feng Guo (Hokkaido University), Osamu Fujita (Hokkaido University)

This paper experimentally reveals the spread rate of flame over electric wire placed in a cylinder with various inner diameters, given various flow velocities. The objective of this study is to clarify the effects of size of the space and air velocity on the electric wire insulation burning. This is new in view of that previous works about such enclosure effect are mainly focusing on the flat material such as flat PMMA samples, cottonfiberglass fabric, and Cellulosic paper. Sample wires were LDPE-coated copper and nichrome wires. The experiments were performed under atmospheric pressure conditions. The results showed that for copper wire, the flame spread rate increases with tube diameter and flow velocity. For the nichrome wire, the trend was the same as that for copper wire in the small-diameter region, but in the large-diameter region, the flame spread rate increased as the flow velocity slowed down. These results may be attributed to the local oxygen concentration of the gas flowing to the flame and the flame inclination angle at the high flow velocity.

Paper ID: 244

A tri-variate extension of the moment projection method for multicomponent particle formation and evolution

Tongtong Yan (Shanghai Jiao Tong University), Zhiwei Zhao (Shanghai Jiao Tong University), Shaohua Wu (Dalian University of Technology), Dezhi Zhou (Shanghaijiaotong University)

Properties and performance of functional materials synthesized in flames are highly dependent on the properties of particle composition. This study develops a new method of moments, called tri-variate extension of the moment projection method (TVMPM) to consider any three internal coordinates of particles such as volume, surface area and component mass for multicomponent particle formation and evolution in flames. Constant kernel is used to verify the validity of TVMPM and avoid interference from other factors. And in order to obtain the weights and abscissas for a set of moments, a three-dimensional Blumstein and Wheeler algorithm is constructed. An advantage of the TVMPM is that the number of smallest particles can be directly tracked, which makes it possible to close the shrinkage and fragmentation terms. After the corresponding high-order moments are obtained by TVMPM, they are compared with the moments obtained by the direct simulation algorithm to verify the reliability of the method. The results show that the TVMPM method has high precision in 3D computation and can save computing resources effectively.

Paper ID: 245

Study on the iron ore sintering process with flue gas recirculation system

Chia-Chen Ho (National Sun Yat-Sen University), Hsu Sheng-Yen (National Sun Yat-sen University), Wai Siong Chai (National Sun Yat-Sen University), Yi-Sung Huang (China Steel Corporation)

This study employs experimental and numerical method to investigate the sintering propagation phenomenon of the process. Experimental results were used in the parameter correction and subsequent numerical model verification. The model successfully simulates the combustion heat release of fine coke, thermal cracking of limestone, evaporation and condensation of water, as well as movement of high-temperature areas in the sintering material layer. The relationship between the flow velocity and the pressure difference caused by the material layer such as material at different heights, and the measurement results are used to find out the parameters of the pressure loss of the porous medium by the linear regression method. A maximum of 10% energy conservation is estimated to be achieved with current flue gas recirculating (FGR) system.

Paper ID: 246

Comparison of the ignition and combustion characteristics of single and tandem cavity Scramjet combustor using a μPDE

Min-Su Kim (Pusan National University), Jae-Hyuk Lee (Pusan National University), Inhoi Koo (Pusan National University), Eun-Sung Lee (Pusan National University), Hyung-Seok Han (Pusan National University), Jeong-Yeol Choi (Pusan National University)

Ignition and combustion characteristics of tandem cavity scramjet combustor were investigated using a direct-connect scramjet combustor(DCSC) and a micro-pulse detonation engine (μPDE). High enthalpy supersonic air was supplied to the scramjet combustor at Mach number 2 and total temperature of 1,000 K by a vitiated air heater(VAH). The scramjet combustor consists of an isolator and a combustor with rectangular cross-section. Two cavities were installed at the upper wall of the combustor. A μPDE was installed above the cavity to propagate the detonation and high temperature plume into the recirculation zone of cavity. The combustion characteristics were investigated using wall pressure profiles and high-speed camera snapshots of Schlieren imaging. According to the equivalence ratio and the location of the μPDE, a total of six cases were performed three times each. The scramjet combustor was ignited by the μPDE under all conditions. In the case of a relatively high equivalence ratio, jet-wake and cavity shear-layer flame transition mode is created. When the position of the μPDE was changed, the result showed that the flame development and attachment position changed according to the equivalence ratio.

Paper ID: 247

Optimization of computational fluid dynamics solver on parallel computing systems

Donghyuk Shin (Korea Advanced Institute of Science and Technology), Mert Yakup Baykan (Korea Advanced Institute of Science and Technology), Inyeong Gu (Korea Advanced Institute of Science and Technology)

In this research, we aim to optimize a computational fluid dynamics (CFD) solver on a parallel computing system by investigating the effect of compiler and message passing interface (MPI) selection on the performance of the CFD code. Our preliminary findings show that the Mvapich2 package with GNU Compiler Collection (GCC) improves the speed of the CFD code by around 5% compared to the OpenMPI package with GCC. The simulation results using the two packages show little discrepancies that need further investigation.

Paper ID: 248

Development of global combustion mechanism of NH_3 for computational fluid dynamics on cofiring with pulverized coal

Woosuk Kang (Sungkyunkwan University), Jongmin Park (Sungkyunkwan University), Changkook Ryu (Sungkyunkwan University)

NH_3 cofiring with pulverized coal has recently emerged as a new measure for CO_2 emission reduction by displacing fossil fuel in a coal-fired power plant. It requires the optimization of cofiring method to achieve a low NOx emission without deteriorating the combustion efficiency and boiler performance. In the optimizing process, the use of computational fluid dynamics (CFD) is essential by evaluating different cofiring methods and modifying burner designs of a boiler. However, the detailed reaction mechanism of NH_3 is not directly compatible with the existing reaction schemes of pulverized coal which significantly simplify the coal combustion. This study developed a global combustion mechanism of NH_3 for CFD applications to cofiring with pulverized coal using an optimization algorithm. Based on a detailed reaction mechanism of NH_3, the key reaction parameters were acquired for different temperatures (1500−1900 K) and equivalence ratios (0.9−1.4) using Chemkin-Pro: i) characteristics time for decrease in NH_3 concentration, ii) final N_2O concentration, and iii) final NO concentration. Using the results as the reference data, the rate constants for five reactions involving only the major species were optimized by the modified gradient descent method. The optimized global mechanism of NH_3 provided reasonable agreement with the detailed mechanism in terms of the three reaction parameters for the entire reaction conditions.

Paper ID: 249

On the solution of stiff odes with different initial conditions by Fourier neural operator

Yuting Weng (Shanghai Jiaotong University), Dezhi Zhou (Shanghai Jiaotong University)

In this paper, the approach of Fourier Neural Operator (FNO) is applied on stiff chemical kinetic systems to solve ODEs with various initial conditions. Fourier Neural Operator (FNO), as an operator learning method, can model the mapping relationship between solution functions and different initial conditions in a neural network and it is a great method to solve ODEs with different initial conditions. In this paper, FNO is applied to some stiff chemical kinetic systems including ROBER problem and its results are compared with traditional deep neural network under the condition with or without specific sampling method. Finally the results shows that FNO can reach a better precision rate compared with traditional DNN and use less time in training. The approach of FNO is proved to be accurately solve stiff chemical kinetic systems with different initial conditions, promising to be applied for stiff chemical kinetic problems.

Paper ID: 250

Effects of fuel injection strategy and ammonia energy ratio on combustion and emissions of ammonia-diesel dual-fuel engine

Shouying Jin (Tianjin University), Binyang Wu (Tianjin University), Zhenyuan Zi (Tianjin University), Puze Yang (Tianjin University), Taifeng Shi (Tianjin University)

The ammonia-diesel dual-fuel (ADDF) engine is an effective way to reduce greenhouse gas (GHG). Aiming

at achieving high thermal efficiency and low emissions of ADDF engine, the effects of ammonia energy ratio (AER) and injection strategy on combustion and emission characteristics were studied by combining experimental and simulation results. It was found that as the AER increased from 0% to 90%, the gross indicated thermal efficiency (ITEg) decreased continuously. Due to the slow flame speed of ammonia and the inhibition of the dehydrogenation process during the low temperature reaction of diesel, the emission of unburned ammonia increased significantly. Amino groups have a denitrification effect, and nitric oxide (NO) can be reduced to more stable nitrogen (N_2). The production and consumption of nitrous oxide (N_2O) were influenced by temperature, and its production region was mainly the low temperature region where the reaction of ammonia occurred. The double injection strategy can significantly improve the activity of the mixture, accelerate combustion, reduce unburned ammonia emissions and incomplete combustion losses. By optimizing the injection strategy and regulating the combustion process, an ITEg of 49.18% can be achieved when the AER was 50%, and GHG can be reduced by 14.2%.

Paper ID: 251

The experimental analysis of the burning characteristics of electrically controlled solid propellant

Daehong Lim (Seoul National Univeristy), Gnanaprakash Kanagaraj (Indian Institute of Technology Hyderabad), Rajendra Rajak (Seoul National University), Jack J. Yoh (Seoul National Univ Korea)

Electrically controlled solid propellant (ECSP) system has been introduced due to its potential in thrust regulation. However, the type of metal additives in ECSP directly affects the burning rate of the propellant thereby the thrust. Present study investigates the burning characteristics of two metalized samples composed of electrically controlled solid propellant combined with 5% (M5) and 15% (M15) (%wt) Tungsten (W) as metal additive. The burning characteristics of ECSP with addition of tungsten was studied through electric signal, flame temperature, and high-speed images. From the electric signal analysis, the two distinct regions were observed: the transient and steady regions. In the transient region, the current and voltage remained almost constant, whereas in the steady region, the current increased linearly for both the metalized samples. When the ongoing burning process belonged to the transient region, intermittent burning was detected, whereas when the process belonged to the steady region a steady downward burning was observed. The flame temperature for both the sample exhibited different burning characteristics, for instance a higher power was required to maintain the combustion of M5 sample, and the flame temperature of the sample was higher. However, as the metal content increased by 15% (M15), the flame temperature decreased by 9%. This is because of the change in metal oxidation with increase in metal content in baseline composition of ECSP. Further it is observed that, the exothermic reaction temperature range of the M5 sample was narrower than that of M15. Therefore, it could be inferred that the increase in metal content in ECSP could cause a transition in the burning characteristics due to its molecular characteristics.

Paper ID: 252

Single pellet combustion of torrefied elephant dung

Yan-Ru Wang (National Cheng Kung University)

In this study, the torrefied elephant dung was characterized by single pellet combustor which it was used to record the combustion time and flue gas emission at different temperature. The influence of ambient

temperature and type of dung (raw and torrefied one) on combustion behavior were conducted in the single pellet combustion. The total combustion time for both fuels were reduced as temperature raised.

Paper ID: 253

Horizontal seismic effect on upward flame spread

Jui-Sen Liao (National Kaohsiung University of Science and Technology), Tzu-Yan Tseng (National Kaohsiung University of Science and Technology), Kuang-Chung Tsai (National Kaohsiung University of Science and Technology)

Earthquakes and fires can occur simultaneously. The study used a vibrator to explore the effect of horizontal earthquakes on wall fires with and without sidewalls. The amplitude and frequency of the vibrator can be adjusted to simulate earthquakes of different seismic intensity scales up to 6 Upper. Specimens used were 0.5 m tall PMMA slabs. The parameters investigated included the height of flame, heat feedback and flame spread rate, while the first two parameters determine the flame spread rate. The velocity of air movement was measured to understand the influence of horizontal vibration on air entrainment. Moreover, the effect of sidewalls was studied. Results show that the flame height without sidewalls was slightly increased with horizontal seismic intensity scale. However, the heat feedback and flame spread rate were decreased with the seismic intensity. Clearly, the effect of increased flame height was suppressed by decreased heat feedback. In the cases with sidewalls, the trends of heat feedback and flame spread rate were consistent with the cases with sidewalls. The only exception was that the flame heights were not influenced by the vibration. Additionally, the vibration enhanced the air entrainment. Conclusively, the horizontal vibration decreased the upward flame spread rate.

Paper ID: 254

Influence of wind speeds and heating exposures on the thermal insulation of intumescent fire-retardant coatings

Saiya Feng (Central South University), Yuhao Li (Central South University), Zhengyang Wang (Central South University), Chuangang Fan (Central South University), Liang Yi (Central South University)

The standard fire resistance test failed to consider the effect of wind on intumescent fire-retardant coatings. This study investigated the thermal insulation of intumescent fire-retardant coatings under various heating exposures and wind speeds. Fire-retardant coating presented a non-uniform intumescent process with wind influence. Wind slowed the initial swelling rate, decreased the maximum coating thickness, and promoted the coating thickness decline. The coating at the front end was shorter than the rear end, which caused a higher steel temperature at the front end. The time of the steel temperature to reach the critical temperature was advanced indicating a decreased thermal insulation. Wind caused a higher coating temperature and accelerated the coating depletion at the front end. The influence is stronger with higher heating exposure and faster wind speed. Wind affects the coating temperature and coating thickness via convective cooling and char oxidation, and char oxidation is a more dominant factor. Empirical correlations were applied to represent the influence of wind on the maximum swelled thicknesses and average swelling rates of fire-retardant coatings at the front end. The predicting equation indicated the synergistic effects of wind speed and incident heat flux on the thermal insulation of fire-retardant coating.

Paper ID: 255

Global quench of centrally-ignited premixed ammonia/air flames by turbulence

Yi-Rong Chen (National Central University), Tinh Van Mai (National Central University), Hao Yu Hsieh (National Central University), Shenqyang S Shy (National Central University)

Global quench (GQ) of centrally-ignited, outwardly expanding premixed ammonia/air flame kernels by turbulence is explored in a fan-stirred cruciform burner capable of generating near-isotropic turbulence over wide ranges of r.m.s. turbulence fluctuation velocities (u'=0-8.4m/s). Ignition is via pin-to-pin stainless-steel electrodes using a range of a well-controlled ignition energy (E_{ig}=50-500 mJ). Interactions of flame kernel and turbulence over a range of the equivalence ratio (ϕ=0.7-1.2) are recorded by a high-speed camcorder to determine the required critical u'_c for GQ, depending on E_{ig} and ϕ. Results show that GQ depends on E_{ig}; the higher E_{ig} is, the larger u'_c is. Specifically, when ϕ=1, u'_c ≈1.25 m/s when using E_{ig}=50 mJ, while u'_c ≈1.85 m/s when E_{ig}=500 mJ. Further, the highest u'_c ≈2.08 m/s occurs at ϕ=0.9 for GQ of premixed ammonia/air flames, although the largest laminar flame speed S_L=7.95 m/s and the smallest laminar flame thickness $delta_L$=1.82 mm occur at ϕ=1.1. Moreover, turbulent Karlovitz (*Ka*), Markstein (*Ma*), and Lewis (*Le*) numbers are used to explain these results. We find that critical values of $Ka_c=(u'_c / S_L)1.5(L_I/delta_L)$^-0.5 vary drastically from 67/69 at ϕ=0.7/0.8 with *Ma*<0 or *Le*<1 to 21/12 at ϕ=1.1/1.2 with *Ma*>0 or *Le*>1, where L_I is the integral length scale of turbulence.

Paper ID: 260

The effect of dual-wavelength selection on the temperature measurement by two-color pyrometry for coal combustion in premixed methane/air

Ming-Wei Dai (NCKU)

As science and technology develop, people enhance the material standard of living, and those problems will influence energy distribution. According to the distribution of energy in the whole world, in recent years, coal has increased amplitude more than other energy. The goal of zero-carbon emission is yet to be accomplished since hydrocarbon fuels are the main cause of air pollution and global warming. This study investigated the coal combustion during the co-firing and developed a technique for measuring the solid fuel temperature with coal particles in the flame field. The name “Two-color pyrometry” originates from using two wavelengths, as burning the coal particles would emit the filters, which can measure the pulverized coal particle temperature. In Two-color pyrometry, two wavelengths of thermal radiation were emitted by incandescent soot particles and measured as temperatures. A hybrid flame contained methane (CH_4)/air/coal premixed flames.

Paper ID: 262

Micro-pin-fin heat sink design with flow normalization

Jer-Huan Jang (Ming Chi University of Technology), Syed Masihuzzaman (Ming Chi University of Technology)

The micro-pin-fin heat sink (MPFHS) is commonly used to improve heat transfer for microelectronic devices. The heat transfer improvement with flow normalization on the micro-pin-fin heat sinks has been numerically investigated in this work. The flow normalization is achieved by changing the diameters of micro-pin-fins. Therefore, two types of micro-pin-fin arrangement have been investigated in this work: straight micro-pin-fin

heat sink (S-MPFHS) and straight variable diameter micro-pin-fin heat sink (SVD-MPFHS). The solid part of the micro-pin-fin heat sink is made of copper and the coolant is liquid water. Commercial software, Ansys-Fluent, has been employed for the numerically analysis. It is found that the SVD-MPFHS has better flow distribution in primary channels and higher flow through secondary channels than the S-MPFHS. It is also noted that the maximum and average base temperatures of SVD-MPFHS decreased by 2.63 and 1.22 K, respectively, when compared to that of S-MPFHS. In addition, the Nusselt number of SVD-MPFHS is improved by 4.2%, and the SVD-MPFHS provides better thermofluid performance over the full Reynolds number range examined.

Paper ID: 263

On the application of CH planar laser-induced fluorescence in flame spray pyrolysis

Callum M Kennedy (University of Sydney), Matthew J Dunn (The University of Sydney), Assaad Masri (University of Sydney)

This work presents a novel application of 10 kHz CH planar laser-induced fluorescence (PLIF) to a flame spray pyrolysis (FSP) flame. The measurements provide preliminary information about the reaction zone and a proof of concept for the application of CH PLIF in similar low-density spray flames. Further analysis is provided with respect to OH PLIF and Mie scattering. OH PLIF is operated in the linear regime and is intended as a qualitative metric to visualize high-temperature flame regions. Mie scattering contextualizes the droplet field in FSP flames and is primary limiting factor in the application of CH PLIF. The droplet field, high-temperature regions of the flame and the reaction zone are of primary importance to understanding the boundary conditions for nanoparticle growth in FSP.

Paper ID: 264

Thermodynamic analysis of ammonia as a blast furnace reductant followed by artificial neural network prediction of blast furnace characteristics with ammonia addition

Paul J Sarles (National Cheng Kung University), Wei-Hsin Chen (National Cheng Kung University)

This study aimed to investigate potential blast furnace operation using ammonia as a reduction agent in supplement to coke for carbon emissions using the minimization of Gibbs free energy method, then to predict the results of the thermodynamic analysis using a neural network. In the thermodynamic analysis, first nominal blast furnace operation was simulated using the composition of Mesabi range iron ore, blast air, coke, and flux. Then, incremental ammonia addition with incremental reduction of the coke charged into the blast furnace was simulated under blast air rich and reduced blast air condition. The simulation results were analyzed for iron composition, enthalpy of reaction, and concentration of carbon monoxide (CO_2), carbon monoxide (CO), and oxides of nitrogen (NOx) in the air at various stages in the blast furnace. The results showed correlation with existing knowledge about blast furnace operation and indicate that ammonia could have similar challenges as those which exist for hydrogen as a supplemental blast furnace fuel. The results of the blast furnace simulation were then used to develop a neural network to predict blast furnace analysis parameters based on ammonia addition percent, temperature, and blast air addition.

Paper ID: 266

A deep learning approach to predicting fuel composition effects on exhaust gas composition

Nursulu Ms. Kuzhagaliyeva (KAUST), Inna Gorbatenko (King Abdullah University of Science and Technology), Andre Nicolle (Aramco Fuel Research Center), S. Mani Sarathy (KAUST)

We herein demonstrate the potential of deep learning (DL) techniques for high-throughput assessment of exhaust pollutant mitigation. Building upon linear mixing operator (MO) implanted in the network architecture introduced by Kuzhagaliyeva et al [1], we adopt the reported model's architecture to predict formation of five pollutants, including ethylene, propylene, 1,3-butadiene, benzene and carbon monoxide. MO estimates the mixture hidden representation vector as a linear combination of each single components' vectors in a given blend and allows the prediction of pollutant formation propensity for practical fuels, i.e., mixtures. (T, P, ϕ) premixed stagnation flame libraries for 175 mixtures and 73 pure components were generated for model training and validation using state-of-the-art detailed kinetic models for combustion and pollutant formation. To take into account the tabular nature of the generated database, three sampling strategies were explored. We demonstrate that the stratification in sampling with structural data plays a significant role in improving model's generalization capability. The developed DL model exhibits high accuracy of predictions on unseen pure components and blends across all tasks by reaching less than 10% deviations from pollutants formation propensities estimated using 1D flame structure assessment.

Paper ID: 267

Study on combustion characteristics in steam-diluted hydrogen/oxygen multi-cluster burner using PSR and LES

Shan Jiang (Tokyo Institute of Technology), Masayasu Shimura (Tokyo Institute of Technology), Mamoru Tanahashi (Tokyo Institute of Technology)

Combustion characteristics in a steam-diluted hydrogen/oxygen multi-cluster burner are investigated using perfectly stirred reactor (PSR) and large eddy simulation (LES). In PSR, different equivalence ratios and mass dilution rates were applied to study their effects on combustion temperature and radical distribution. It has been revealed that higher mass dilution rates can result in lower combustion temperature and lower radical mass fraction, while mass fractions of most radicals are lower under rich combustion conditions. LES is used to investigate the distribution of streamlines and temperature fields inside the burner. Its results reveal that recirculation zones are created close to the inlet wall, resulting in an enrichment of the hot burnt gas, which may be resolved by applying greater jet inclination angles.

Paper ID: 268

Experimental study of oxy-flames in a coaxial dual-shear jet burner

Kuanyu Wang (BIT), Xie Dingjiang (Beijing Institute of Technology), Qing Cao (Beijing Institute of Technology), Yong Tang (Beijing Institute of Technology), Baolu Shi (Beijing Institute of Technology)

This work aims to study oxy-combustion technology which can be combined with carbon capture and storage (CCS) technique for zero carbon emission, First, a coaxial dual-shear jet burner is designed for stable non-premixed methane/oxygen combustion. Two group tests involving various flow rates and reactants-feeding methods are conducted. The flame images show that two reaction surfaces are formed along the two shear

layers. Compared with traditional coaxial jet flames, the heat release indicated by OH* intensity is lower near the nozzle exit while it is more concentrated downstream at large flow rate conditions. Besides, the position where the OH* intensity reaches the maximum moves upstream over 1/3, which infers a considerable decrease in the stoichiometric mixing length. However, temporal variations of flame structure and acoustic pressure fluctuation (APF) occur at low flow rate conditions. The high-speed photograph measurements reveal that the fluctuation frequency of the flame structure (about 333 Hz) is approximately equal to the primary frequency of the APF (330 Hz). Moreover, the frequency with the highest amplitude is close to the acoustic resonant frequency in the combustion chamber. It demonstrates that the flame oscillation is probably the longitudinal mode.

Paper ID: 270

Comparison between decomposition kinetics of mechanoactivated and recrystallized ammonium perchlorate composite solid propellant

Sairaj Eknath Gaunekar (Indian Institute of Technology Goa)

Ammonium perchlorate is the most widely used oxidizer in composite solid propellants (CSP). Chemical kinetics pertaining to two formulations of propellants consisting of fine recrystallized and fine ball milled ammonium perchlorate respectively was reported here. Thermogravimetry experiments were performed to analyze the decomposition characteristics of the propellants. Friedman isoconversational method was used to obtain the kinetic parameters. The average activation energy obtained for CSP containing recrystallized AP and ball-milled AP was found to be 199±56 kJ/mol and 127.8±22.2 kJ/mol, respectively. Similarly, the log of pre-exponential factor (ln(A)) obtained for CSP containing recrystallized AP and ball-milled AP was 14.6±4.8 ln(1/s) and 8.6±1.8 ln(1/s), respectively. Among some interesting observations that emerged, the decomposition and the reaction rate were higher for the formulations containing ball-milled AP.

Paper ID: 271

Fast catalytic pyrolysis of kraft lignin into monocyclic aromatic hydrocarbons over in-situ generation of Fe-based catalyst

Haoran Liu (Shanghai Jiao Tong University), Yang Shen (Shanghai Jiao Tong University), Yanan Zhu (Shanghai Jiao Tong University), Zhongyue Zhou (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University)

Iron ore was investigated as a potential metal catalyst for kraft lignin without the use of an external solvent. A pyrolysis reactor combined with time-of-flight mass spectrometry (Py-TOF-MS) was used to evaluate the performance of the catalyst. The composition of the pyrolysis products was determined in detail. The catalyst before and after the reaction was characterized using a transmission electron microscope (TEM) to determine changes in structure and elemental distribution during the reaction. The impact of temperature on product distribution was also studied. The best results were obtained at 550°C resulting in 81% of monocyclic aromatic hydrocarbons (MAHs) from catalytic pyrolysis of kraft lignin. Our results clearly reveal that a cheap iron ore catalyst has the potential to be used for the pyrolysis of kraft lignin for the production of valuable biobased aromatic hydrocarbons.

Paper ID: 272

Study of the pyrolysis characteristics of plastics by soft photoionization mass spectrometry

Hai-Rong Ren (Shanghai Jiao Tong University), Haoran Liu (Shanghai Jiao Tong University), Cunhao Cui (Shanghai Jiao Tong University), Yanan Zhu (Shanghai Jiao Tong University), Zhongyue Zhou (Shanghai Jiao Tong University)

Transforming waste plastics into clean fuels by pyrolysis is conducive to environmental protection, and also helps to alleviate the energy crisis. Therefore, it is necessary to study the pyrolysis characteristics and products of waste plastics. Photoionization time-of-flight mass spectrometry (PI-TOF-MS) uses VUV lamps as ionization source, resulting in less ion fragments, which is conducive to the detection of products distribution in the process of plastic pyrolysis. In this paper, thermogravimetry and PI-TOF-MS were combined to study the pyrolysis curves of PE and PVC under different heating rates and different gas atmospheres, and the pyrolysis products of PE and PVC were detected online. The pyrolysis temperature range of PE is 388℃~529℃, and the decomposition products mainly include propene, butene, pentadiene, hexadiene, octene and so on. The pyrolysis temperature range of PVC is 242℃~557℃, including two stages, and the mass of the residue is 7.2% of the initial mass. The pyrolysis products of PVC mainly include benzene, toluene, ethylbenzene, naphthalene, 1-Methyl-Naphthalene and so on.

Paper ID: 273

A study of pressure dependences of intermediates towards the low-temperature oxidation of n-heptane by synchrotron photoionization mass spectrometry

Weiye Chen (University Of Science And Technology Of China), Qimei Di (University Of Science And Technology Of China), Hao Lou (University Of Science And Technology Of China), Jiuzhong Yang (University Of Science And Technology Of China), Zhandong Wang (University Of Science And Technology Of China)

Pressure is one of the important factors to affect combustion chemistry process, which can determine the reaction rate rules of some key reactions and regulate the branching ratios of different reaction channels in low-temperature autoxidation. It is significant to understand the pressure-dependent effect of oxidation intermediates and explore the potential driving force of pressure-dependence from reaction mechanism, which is helpful to provide guidance for the development and improvement of theoretical models. In this work, 0.25% n-heptane with equivalence ratio of 1 and residence time of 2 sec has been performed in low-temperature oxidation environment at three different pressures. The results have been shown in two-dimensional views of mole fraction profiles associated with temperature and pressure. Intuitional influences of pressure-dependent effect to fuel conversion have been revealed. Various pressure-dependent effects are observed by the mole fraction profiles of active intermediates, i.e., peroxides, organic acids, olefins, cyclic ethers, and ketones. Combined with chemical kinetic model, their formation pathways are used to explain the causes of pressure-dependent effects, including variation of branch ratio of different competitive channels with pressure.

Paper ID: 275

Numerical analysis of fuel evaporation and mixing in a passive pre-chamber methanol opposed-piston engine

Rafael Menaca (King Abdullah University of Science and Technology), Mickael Silva (KAUST), Kevin Moreno-Cabezas (KAUST), Giovanni Vorraro (KAUST), James W.G. Turner (KAUST), Hong G. Im (KAUST)

Opposed-piston two-stroke engines (OP2S) have remarkable high thermal efficiencies and fundamental advantages over four-stroke conventional diesel engines. Therefore, combining this concept with renewable fuels and advanced technologies, such as pre-chambers, can help in the transitions to high-efficiency carbon-neutral powertrains. Key engine design aspects contributing to methanol vaporization and mixture formation in a passive pre-chamber OP2S engine were investigated numerically. CONVERGE^{TM} was selected as solver to explore the sensitivity of the vaporization and the mixture formation to the variation of injection direction and the swirl angle. The swirl angle has been scarcely documented in OP2S engines and previous studies show that its implementation generates a concentration of hot remaining gases around the cylinder axis. Specific to methanol, these residuals could possibly enable a higher vaporization. However, this study shows that the vaporization is more sensible to the turbulent kinetic energy than the flow patterns or the remnant combustion products.

Paper ID: 276

A comparative tank-to-wheel life cycle assessment of hydrogen fuel cell electric, internal combustion engine, and battery electric buses operating in Saudi Arabia

Chengcheng Zhao (King Abdullah University of Science and Technology), Leiliang Zheng Kobayashi (King Abdullah University of Science and Technology), Awad Alquaity (KFUPM), Noliner Miralles (Saudi Public Transport Company), S. Mani Sarathy (KAUST)

Proton exchange membrane (PEM) fuel cell vehicles (FCVs) offer a potential solution for decarbonizing the heavy-duty transportation sector. This study provides a comprehensive tank-to-wheel life cycle comparison of PEM FCV to battery electric vehicles (BEVs), and conventional internal combustion engine vehicles (ICEVs) for bus applications in terms of energy consumption and emissions according to the methodologies based on the DIN ISO 14040 and 14044. The well-to-tank aspects of fuel/electricity production are not included in this work. Emissions and energy consumption were calculated for all stages of the buses' life cycle, which includes the raw material extraction, vehicle material production, vehicle material transport, vehicle assembly, vehicle transport, vehicle operation, vehicle disposal, and recycling phases. Considering the entire vehicle cycle, ICE buses (ICEBs) have the highest energy consumption and greenhouse gas (GHG) emissions with a lifetime of 508,080 km for 10 years, while the hydrogen PEM fuel cell buses (FCBs) have the lowest GHG emissions, and the battery electric buses (BEBs) have the lowest energy consumption.

Paper ID: 277

Development of three-feed stream steady laminar flamelet model in OpenFOAM: assessment for a reacting jet issuing into a hot and diluted coflow

Danh Nam Nguyen (Ulsan National Institute of Science and Technology), Chun Sang Yoo (Olsan National

University)

A three-feed stream steady laminar flamelet model has been implemented in OpenFOAM as a part of the development of a numerical framework for simulations of non-premixed flames under transcritical and supercritical conditions (i.e., in rocket engines or in direct fired supercritical carbon dioxide gas turbine combustors). The developed code is adopted to simulate a reacting jet issuing into a hot and diluted coflow (i.e., HM3 flame) with RANS approach. A good agreement observed in the comparison of available experimental data and previous studies with data obtained from the present study proves that the implementation of the model is proper, and the developed framework can be used for turbulent non-premixed flames with a reasonable computational cost. This is an important step toward the development of the three-feed stream steady laminar flamelet model for reacting flow simulations under high pressure conditions.

Paper ID: 279

Risk assessment and fire dynamics simulation of ammonia as a fuel use in combined cycle power plants

Heekyung Park (Incheon National University), Min Chul Lee (Incheon National University), Dae Jin Jang (Incheon National University), Seungyeon Jeong (Incheon National University), Seokhui Lee (Incheon National University)

This study shows a quantitative risk assessment for the boiling liquid expanding vapor explosion, one of the fire explosions of aqueous ammonia. Case of ammonia, among alternative fuels, the damage effects and risks were caused by radiant heat in leakage accident. To investigate the risks in advance and for safety operation, quantitative risk assessment using numerical analysis tools, ALOHA and Pyrosim, were conducted. Analysis tools can prepare for accidents by keeping a separation distance.Thus, by analyzing various accident risk scenarios, contribute to the application and development of safety carbon-free fuels technology.

Paper ID: 280

Experimental study on pyrolysis and combustion properties of insulation materials

Yejin Ha (Pukyong National University), Joonho Jeon (Pukyong National University)

Fire accidents caused by combustible insulation material used as a core of sandwich panel occur almost every year, resulting in serious human and property damage. In this study, expanded polystyrene and polyurethane foam corresponding to organic insulation and glass wool corresponding to inorganic insulation were selected to analyze the pyrolysis and combustion properties of each type of the insulation material through experiments. For the TGA experiment, the heating rate was changed to 5, 10, 15, 20 ℃/min to examine the effect of heating rate on the pyrolysis of solid material. In the smoke density chamber experiment, the heat flux was changed to 25, 50 kW/m2 to examine the effect of heat flux on the smoke density of insulation materials. In this experimental study, it could be used to provide input data required for simulation before accurately predicting the pyrolysis and combustion behavior of solid combustible materials using FDS model.

Paper ID: 281

The experiment and numerical investigations on hydrogen production from ammonia cracking: a priori study

Danh Nam Nguyen (Ulsan National Institute of Science and Technology), Jae Hun Lee (UNIST), Hae Won Seo (Research Institute of Industrial Science & Technology), Hyung Jun Ahn (Research Institute of Industrial Science & Technology), Beom-Sik Kim (Research Institute of Industrial Science & Technology), Chun Sang Yoo (Ulsan National University)

The characteristics of ammonia cracking using Ru/Al_2O_3 catalyst to produce hydrogen are experimentally and numerically investigated by varying temperature of the furnace (450-600℃). The experimental results show that more than 90% of ammonia is converted into hydrogen if the temperature of the catalytic reactor is above 490℃ (furnace temperature is 550℃). The successful implementation of the Takahashi's chemical kinetic model [1,2] in Arrhenius form is a crucial step in making the model to be applicable in different numerical frameworks using CHEMKIN format (e.g., ANSYS Fluent [3], OpenFOAM [4] etc.,). In addition, a good agreement in the ammonia conversion rate between experiments and simulations for the Ru/Al_2O_3 catalyst in this study implies that the Ru-based Takahashi's chemical kinetic model can be a good option for the simulations of ammonia decomposition using Ru/Al_2O_3 catalyst in the context of lacking a chemical mechanism.

Paper ID: 282

The effect of immersed metal objects on burning rate of in-situ burning

Jun Jia Ye (National Kaohsiung University of Science and Technology), Tzu Yan Tseng (National Kaohsiung University of Science and Technology), Kuang-Chung Tsai (National Kaohsiung University of Science and Technology)

In-situ burning (ISB) is effective to deal with the spill oil accidents. However, the burning on water results in huge thermal loss and poor burning efficiency, lowering the burning rate. This study consequently aimed to improve the burning rate of ISB by using immersed metal objects. Different types of metal objects and different immersed depths were investigated. Clearly, the presence of metal objects enhanced the burning. The flame with the immersed mesh at liquid surface was higher than that without metal objects for 22%. The mass loss rate with the immersed mesh was 21% higher than that without the metal objects. The addition metal objects could provide extra heating resource and the subcooled nucleate boiling also performed at the lower surface of the immersed metal objects to induce more bubble generation.

Paper ID: 283

High-speed deflagration in narrow channels at cryogenic temperatures

Canruo Chen (Tsinghua University), Damir Valiev (Tsinghua University)

A supersonic deflagration is numerically investigated in narrow channels with walls maintained at cryogenic temperatures. Low-speed steady and high-speed quasi-steady regimes of deflagration are obtained. For the latter, the measured deflagration velocity is close to CJ deflagration velocity. The observed maximum pressure during the high-speed deflagration at cryogenic temperatures can reach up to 40 times higher than that at an ambient temperature. Quasi-steady high-speed deflagrations are characterized by pulsations of velocity; a

periodic emergence of two discrete shock waves is observed via numerical Schlieren imaging.

Paper ID: 284

Understanding the thermal behaviour of electrically controlled solid propellant with different metal additives

Rajendra Rajak (Seoul National University), Daehong Lim (Seoul National Univeristy), Gnanaprakash Kanagaraj (Indian Institute of Technology Hyderabad), Jack J. Yoh (Seoul National Univ Korea)

Electrically controlled solid propellant (ECSP) has been investigated from past many decades but not enough effort has been given to understand the physio-chemical mechanism of the ECSP burning and thermal behaviour on addition of different metal additives. This paper enunciates the effect of different metal additives viz. Aluminium(Al), Magnesium(Mg) and Titanium(Ti) mixed in the ECSP baseline composition, with lithium perchlorate (LP) as the oxidizer and polyvinyl alcohol (PVA) as binder. Addition of different metals affects the thermal stability of the ECSP combustion. ECSP with three different metal additives was synthesized and the burning experiments of each sample under atmospheric condition were done to understand the flame behaviour. Thermal analysis using differential scanning calorimetry (DSC), thermogravimetric analysis (TGA) reveals the thermal stability and associated mass loss of the considered ECSP's. It is noticed that the decomposition of the Mg based ECSP occurs at higher temperature range as compared to Ti and Al based ECSP. Surface morphology of the aforementioned composition were observed and their elemental mapping using EDS was conducted. It is noticed that the lithium perchlorate- polyvinyl alcohol based baseline composition is not the universal composition to accommodate any metal additives, furthermore the burning ceases when the magnesium is added to the baseline.

Paper ID: 287

Development of a 200 kgf pre-decomposition hydrogen peroxide hybrid rocket

Chia-Wei Chang (National Cheng Kung University), Hung-Wei Hsu (National Cheng Kung University), Hong Yuan Li (National Cheng Kung University), Yei-Chin Chao (National Cheng Kung University)

In a pre-decomposition hydrogen peroxide(HP) hybrid rocket, a catalyst bed mounted before the combustion chamber decomposes HP into hot gases which ignite the fuel without additional ignition devices. That makes pre-decomposition HP hybrid rockets great potential to be upper stage rockets. The decomposition rate of HP is critical to ignition. The injector developed in this study can constrain HP flow rate overshoot to about twice of the steady flow rate and distribute it evenly. With the proper injector design, the catalyst filling amount that leads to bed pressure drop is reduced and the catalyst bed decomposes HP into the gases reaction region right after the valve opening. By experimental verifying, the catalyst bed reaction time in this study tends to be stable(~0.44s) and is very close to the 50P fuel grain engine ignition delay time. Compared with the 300kgf

system invented in our laboratory in the past, the life of the catalyst bed in this study is prolonged by at least three times and is still able to work smoothly. This study also verifies using HP decomposition gases flow to insulate the swirler from the central recirculation zone can prevent the ablation. Eventually, a 200kgf Pre-decomposition HP Hybrid Rocket is successfully developed.

Paper ID: 288

A direct numerical simulation study on spherically expanding liquid ammonia flames

Zhenhua An (Kyoto University), Jiangkuan Xing (Kyoto University), Ryoichi Kurose (Kyoto University)

Directly using liquid ammonia in combustion devices can make the fuel supply system simpler and reduce equipment costs. Recently, there are several studies reported that liquid ammonia combustion was realized in gas turbine and internal engine conditions, and pointed out that preheating the carrier gas or blending the methane can improve the stability of liquid ammonia flames. However, more detailed explanations for the ignition, propagation, and stability of liquid ammonia flames are still lacking. Therefore, this study investigated the spherically expanding mechanism of liquid ammonia flames in different initial temperatures using direct numerical simulation (DNS) coupled with detailed chemistry. Three pure gaseous/liquid ammonia cases with the initial temperature of 300 K and 500 K were compared. The results showed that pure liquid ammonia outwardly expanded and the reaction rate was significantly promoted after preheating.

Paper ID: 289

Can we compare different façade fire standards fairly?

Yizhou Li (The Hong Kong Polytechnic University), Zilong Wang (The Hong Kong Polytechnic University), Xinyan Huang (The Hong Kong Polytechnic University)

Façade fire is becoming a global problem in high-rise buildings. However, façade fire standard tests vary from country to county bring some significant problems and misunderstandings when there is no common recognition among different countries. This study first briefly reviews the scenario-based façade fire standard tests, such as GB/T 29416-2012 (China), BS-8414-1: 2015 (UK), ISO 13785-2, NFPA 285-2019 (USA), and JIS A 1310 (Japan). This study mainly focuses on the behaviors of the spilled flame in five façade fire standard tests and aims at finding the similarities and differences among these standard tests. Under the default fire scenario, the BS 8414-1 and GB/T 29416 generate the largest heat flux (~100 kW/m^2) to ignite the facade above the opening. The facade fire plume in ISO 13785-2 produces a near-constant heat flux (~50 kW/m^2) for 2 m above the opening. The heat flux of NFPA 285 largely depends on the extra window burner, and JIS A 1310 can produce intensive heating on the facade by increasing the chamber fire heat release rate (HRR). The study explores the equivalent heat flux for different standard tests that lead to a fair comparison.

Paper ID: 290

Investigation of near-wall turbulent prediction for burning-off removal process of carbon deposits on coke-oven walls

Yi-Da Chung (National Cheng Kung University), Keh-Ching Chang (National Cheng Kung University)

The near-wall treatment approach plays an important role in accurate turbulent flow simulation, particularly for predicting the heterogenous reactions on the wall in the coke oven chamber. In the study, two near-wall treatments, including the Enhanced Wall Treatment based on k-ε RANS model and the blended SST k-ω model (the nearest grids to wall being within $0 < y^* < 1$) that bridge the fully turbulent subregion to the near wall subregion, were studied in the burning-off simulation for removing carbon deposits on walls in the coke oven chamber. The burning-off processes under two mass flow rates of the inserted air injection pipe, 5000 and 20000 LPM were simulated. The comparison between the results obtained respectively with each turbulence

model shows that the use of proper near-wall layout in the computational mesh is necessary in the simulation of combustion process associated with the heterogeneous reactions on wall such as the present study. It affects the predictions of not only the carbon removal rate but also the mean frequencies of quasi-periodic inhale-exhale phenomena observed at four open inlets. It is therefore suggested that the blended SST k-ω model has to be used in the simulation of the present physical problem.

Paper ID: 291

Mesoscale modeling of deflagration on the surface of metalized solid fuels

Hong-Suk Choi (Seoul National University), Jack J Yoh (Seoul National University)

This study examines mesoscale deflagration, a propagating flame that forms on the surface of a metalized solid propellant. Energy transfer to the adjacent material occurs via convection and diffusion, which are separately handled based on the associated time scale. For convective and diffusive burning, the Arrhenius law is utilized, along with the third order Runge-Kutta method and Essentially Non-Oscillatory (ENO) schemes to discretize the temporal and spatial domain. The interface between two materials is tracked by the level-set function which describes the deforming boundary. The unreacted particles are ignited by the strong compression wave in the convection dominating region while the conduction governs the heat flux in the reaction zone. In particular, the slow flame that includes conductive transfer of heat is handled independently from convective transfer via a large time step scheme. The flame velocity in the simulation is compared to the theoretical value based on the pressure burn rate. Furthermore, the melt layer where the surface burning occurs is reproduced to elucidate the process of surface reaction between the unreacted propellant and exhausting gas

Paper ID: 292

Surface dynamics of CeO_2-supported noble metal catalysts

Zuo Li (The University of Sydney), Mohamed Marei (The University of Sydney), Assaad R. Masri (The University of Sydney), Alejandro Montoya (The University of Sydney)

Noble metals supported on CeO_2 is an effective catalyst for the CH_4 oxidation. The surface morphology is pivotal in the stable catalytic activity under kinetic-limited oxidation conditions. Different synthesis methodologies (calcination and pre-treatment methods) are used to produce the Pt/CeO_2 and Pd/CeO_2 with different surface structures. The surface dynamics during the synthesis and reaction are analysed, and it is determined that the noble metal nanoclusters supported on CeO_2 surface provide the optimum catalytic activity.

Paper ID: 294

Investigation of lean blow-off dynamics of a 2D bluff-body stabilized premixed flame

Xiaoyang Wang (Shanghai Jiao Tong University), Kunpeng Liu (Shanghai Jiao Tong University), Chen Fu (Shanghai Jiao Tong University), Juan Yu (Shanghai Jiao Tong University), Yi Gao (Shanghai Jiao Tong University)

In recent years, the bluff-body stabilized flames have been widely used in practical combustion devices due to their excellent stability performance. However, the mechanism behind the blow-off event of two-dimensional (2D) bluff-body stabilized flames is still unconfirmed. In this study, the lean blow-off (LBO)

dynamics of a 2D bluff-body stabilized premixed flame were investigated. Experimentally, 5 kHz OH* chemiluminescence and the simultaneous 10 Hz particle image velocimetry (PIV) and OH planar laser-induced fluorescence (OH-PLIF) technology were applied. Based on the high-speed OH* chemiluminescence, it is found that a significant change of the flame structure, the "necking" of flame in the stagnation-point region (SPR) followed by "pinch-off" of the flame, is considered a typical precursor of blow-off. The causes of the "necking" and "pinch-off" were analyzed based on the PIV and OH-PLIF under stable and near LBO conditions. Under the near LBO condition, the flame fronts in the SPR move towards the low-velocity region due to the reduced flame speed, and the "necking" of flame appears. In addition, due to the weak "back support" and high stretch rate, the flame in the SPR is the weakest, and the "pinch-off" occurs consequently.

Paper ID: 295

Full-scale tank fires suppression by using combined system of foam and perlites

Shu-Hsuan Wu (National Kaohsiung University of Science and Technology), Tzu-Yan Tseng (National Kaohsiung University of Science and Technology), Kuang-Chung Tsai (National Kaohsiung University of Science and Technology)

A novel fire suppression system, which combines foam and perlites was proposed. In order to evaluate the suppression performance of the system, the fire suppression efficiency with foam system, perlites and the combined system were assessed by using 1 m oil pan. Additional backboard was used to mimic a tank wall. The rate of foam spread on the fuel and perlites surfaces were measured. The re-ignition and burn-back resistance were tested in the full-scale experiment. The results illustrated that the foam, perlites and the combined system performed better than other two in different performance items. The foam system can extinguish the fires. However, second time re-ignition occurred in two of the three tests, and flames burned back soon. Additionally, the perlites system can almost extinguish the fires but some edge fires occurred, and performed good burn-back resistance. The combined system can extinguish the fires and performed good burn-back resistance. However, it cannot prevent re-ignition. Moreover, fire spread on the fuel surface was faster than that on the perlites surface.

Paper ID: 296

G-equation solver development for kinematics of turbulent hydrogen combustions

Juhun Son (Korea Advanced Institute of Science and Technology), Donghyuk Shin (Korea Advanced Institute of Science and Technology)

In this study, a G-equation solver is being developed, which is capable to simulate kinematic and dynamic flame surface behaviors of turbulent hydrogen flames. To resolve the flame surface, the level-set method was employed to establish the G-equation solver. The G-equation was solved by the back-and-forth error compensation and correction (BFECC) numerical scheme, which has the second-order accuracy in time and space. To simulate turbulent flame and flow field, a turbulence inflow boundary condition was used. Random flow generation techniques for turbulent inflow is implemented, and an OpenMP system was used to reduce calculation time. As initial trials, simulations were conducted on the two-dimensional space. Obtained flame surface areas can be used to develop turbulent combustion models. Later, the flame stretch effect is planned to be implemented. Flame transfer functions will be obtained using flame surface areas, which will help solve

the problem of combustion instability of turbulent hydrogen combustion.

Paper ID: 299

Evaluation of optimal operation based on the utilization of renewable energy in smart farm

Jiseon Park (KITECH), Won Yang (KITECH), Yongwoon Lee (KITECH), Jongsup Hong (Yonsei University)

Existing energy system based on centralized power grid has become important related to solve the intermittency problem as the utilization of renewable energy. This study investigated the impact on energy, environment, and economic effect according to the integration of solar in the existing energy system. The energy system is a smart farm, and power consumption was calculated according to summer and winter. The smart farm consists of solar power generation, heat pumps, a wood pellet boiler, a water storage tank, FCU (Fan Coil Unit), and CO_2 supply system. The heat pump supplies the cooling or heating source of smart farm, and the wood pellet boiler is used as an additional heat source in winter. Solar power is primarily used as the power for the operation of the smart farm, and additional power is supplied from central power. Process analysis of the energy system was performed using In-house code. Then, the entire energy system was analyzed according to the change of ambient temperature. Therefore, the inlet/outlet temperature and power consumption were derived through the process analysis. The analysis results of the smart farm were compared to the amount of solar power generation. In addition, the possibility of energy self-sufficiency was evaluated, and the optimal scenario was proposed for the energy management system.

Paper ID: 301

Characterization of latent heat recovery and SOx reduction of flue gas based on the novel FGC system

HyeonRok Choi (Korea Institute of Industrial Technology), Won Yang (Korea Institute of Industrial Technology), YongWoon Lee (Korea Institute of Industrial Technology), Changkook Ryu (Sungkyunkwan University)

The FGC (Flue gas condenser) system has advantage of increasing the energy efficiency by latent heat recovery of the flue gas (~150℃) from the combustion system. In addition, SOx emission of flue gas is reduced under atmospheric conditions. FGC systems are classified into ICC (Indirect Contact Condenser) type and DCC (Direct Contact Condenser) type according to the heat transfer method between flue gas and cold water. In this study, a novel FGC system was developed in connection with ICC type and DCC, and latent heat recovery and desulfurization characteristics were analyzed under atmospheric. In this study, the desulfurization performance was analyzed according to the inlet water content of the flue gas, L/G ratio (Liquid to gas ratio), inlet SO2 concentration, and the Na/S ratio of the additive. Experimental results presents that in the case of ICC, flue gas with high moisture content had high latent heat recovery efficiency and high desulfurization efficiency. In addition, desulfurization efficiency was higher when the L/G and Na/S ratio increased

Paper ID: 302

Numerical simulation of smoke flow in ship fire under pendulum-like motions

Arata Kimura (National Maritime Research Institute), Hideyuki Oka (National Maritime Research Institute), Yasushi Oka (Yokohama National University)

In recent years, fire accidents in the vehicle spaces of pure car carriers and car ferries have occurred. Although smoke flows originated from fire in the vehicle spaces are affected by the existence of complex structural components and ship motions, the appropriate location of a fire detector for early detection taking into account such factors has been little studied so far. Therefore, we conducted fire experiments using a 1/6 scaled deck model and numerical simulations in parallel and discussed the appropriate installation location of fire detectors based on the vertical distributions of temperature and extinction coefficients in the smoke layer with/without ship motions taking into account the ship structural components.

Paper ID: 303

Ignition, spray, and flow characteristics of a five-injector model combustor

Bowen Yu (Shanghai Jiao Tong University / AECC Commercial Aircraft Engine Co., LTD), Dewen Liu (Shanghai Jiao Tong University), Linye Li (Shanghai Jiao Tong University), Tao Chen (Shanghai Jiao Tong University), Liangliang Xu (Shanghai Jiao Tong University), Xi Xia (Shanghai Jiao Tong University), Fei Qi (Shanghai Jiao Tong University)

The ignition and flame propagation in an aeroengine combustor with multi injectors are interested in both academia and industry. In this work, we setup an experimental system with five spray injectors straight aligned in a rectangular combustion chamber. An electric spark igniter is located at the downstream of the central injector to light the fuel (kerosene) spray. A high-speed camera was used to photograph the OH* chemiluminescence to capture the flame propagation during ignition. Firstly, cold experiments (no ignition) are carried out in several cases with the methods of PLIF and PIV using a high repetition rate burst laser. As a result, the velocity field and the distribution of relative droplet size are obtained. Then, in ignition experiments, the relationship between the number of ignited injectors and the fuel-air ratio are analyzed in combination with the spray characteristics and the flow field.

Paper ID: 304

Chemical kinetics study on the reaction of hydroxyl radical with alkenes

Fushimi Ryota (Toyohashi University of Technology), Tatsuo Oguchi (Toyohashi University of Technology)

The second-order reaction rate coefficients for the reactions of OH + 1-butene, OH + diisobutylene, OH + 2,4,4-trimethyl-1-pentene were measured directly by using the laser-induced fluorescence method. The values for OH + 1-butene reaction in the low-temperature range were validated. Especially for diisobutylene and 2,4,4-trimethyl-1-pentene, they are the first obtained rate coefficients experimentally as far as we know. The rate coefficients decrease with increasing temperature in the range which was observed. It was suggested that the OH addition to the double-bonded carbon was promoted by substituting alkyl groups for hydrogen in the CH_2 group.

Paper ID: 305

Minimum oxidizer supply of smouldering combustion in biomass fuels

Yunzhu Qin (The Hong Kong Polytechnic University), Yuying Chen (University of Technology Sydney), Shaorun Lin (University of California Berkeley), Xinyan Huang (The Hong Kong Polytechnic University)

Smouldering combustion is a slow, low-temperature, and flameless process that usually occurs in porous fuels.

The influence of oxygen supply on smouldering propagation is of vital significance but still not fully understood. In this work, we experimentally quantify the minimum oxidizer supply rate to sustain a smouldering combustion in organic peat soil, pine needle and wood chips with a disclosed tubular smouldering reactor. By increasing the airflow velocity through the porous fuels, no propagation, uni and bidirectional propagation phenomena can be observed in all three biomass fuels. Among the three kind of biomass fuels, smouldering in peat soil was found to need the least oxidizer, i.e., an internal airflow of 0.25 mm/s. The pine needle and wood chips need 0.5 mm/s and 0.7 mm/s, respectively. This work provides data support to understand the relationship between minimum oxygen supply for smouldering and the properties of biomass fuels, and advances understanding of the role of oxygen supply in smouldering combustion mechanism.

Paper ID: 306

Numerical investigation on the effect of wall curvature on propulsive performance of rotating detonation engine

Moeno Miyashita (Keio University), Akiko Matsuo (Keio University), Eiji Shima (Keio University), Akira Kawasaki (Shizuoka University), Ken Matsuoka (Nagoya University), Jiro Kasahara (Nagoya University)

In this study, three-dimensional numerical analyses for RDE combustors with different curvatures were conducted to investigate the effect of the curvature of the combustor wall on propulsive performance. The computational targets are the region where the hydrogen-air premixed gas flows in from two rows of injectors set at the bottom, and continuous propagation was achieved by using a periodic boundary. The height of all combustor was set to 40.0 mm, and the radius of curvature at the outer wall was changed in each case. A cylindrical combustor, whose radius of curvature of the outer wall is 10.0 mm, annular combustors, whose radii of curvature were 10 mm, 15mm, and 20 mm, and linear detonation channels, whose width were 5.0 mm and 6.5 mm, were analyzed. A series of simulations clarified that the differences in the stability of the wave propagation and propagation velocity were clarified. In addition, approximately the same propulsive performance can be obtained for annular combustors and linear detonation channels regardless of the curvature or size of the combustor. This suggests that even when the combustor size is increased, there is no decrease in propulsive performance due to the decrease in curvature.

Paper ID: 307

The collateral effects of nitrogen addition to a commercial self-aspirating burner for lowering the NOx emissions from blended hydrogen-natural gas flames

Adam J Gee (The University of Adelaide), Douglas Proud (The University of Adelaide), Neil Smith (The University of Adelaide), Alfonso Chinnici (The University of Adelaide), Paul Medwell (The University of Adelaide)

The pressing issue of climate change and the need to limit our dependence on non-renewable energy has stimulated research into the effects of hydrogen addition to domestic and commercial burners built to run on natural gas. Despite the large body of research on hydrogen combustion, there remains unanswered questions regarding its adoption when blended with natural gas in domestic and commercial applications. Exhaust gas recirculation (EGR) is a popular strategy to reduce thermal NOx emissions without modifying the burner design. However, the co-effects of various inert species on other critical flame characteristics are not fully

understood for practical combustion systems. This research quantifies the effects of nitrogen addition to hydrogen-natural gas blended flames in a commercial self-aspirating burner on NOx emissions, flame visibility and heat flux. This investigation showed nitrogen addition could maintain levels of NOx below that produced by pure natural gas for hydrogen-natural gas blends up to 90 vol% hydrogen but a significant penalty is paid in reductions in radiant heat transfer. Nitrogen addition also reduced flame visibility and lowers OH* chemiluminescence intensity. Alternative fuel additives or implementation methods would be required if nitrogen is to be utilised as a strategy for overcoming the challenges of transitioning to hydrogen.

Paper ID: 308

Study on combustion characteristic and performance optimization of hydrocarbon premixed flames in stainless steel-platinum segmentation reactor

Cheng-Han Lin (National Cheng Kung University), Hsiao-Hsuan Kao (National Cheng Kung University), Yueh-Heng Li (National Cheng Kung University)

This study discusses the combustion performance and optimization of stainless steel-platinum segmentation micro combustors. The combustion processes accompany the generation of entropy which will cause energy loss. Still, the entropy cannot be determined throughout conducting experiments. The insight of entropy in the microreactor needs to be explored with simulation assistance. By analyzing the entropy generation rate, the combustor can be further obtained to determine the combustion performance of the micro combustor. Three different combustor designs have pore numbers 4 and 6 holes designed according to the fixed platinum catalyst area. The pore number of the perforated holes and pore diameter were chosen as 1 mm and 1.5 mm to investigate the effect on combustion performance.

Three kinds of microreactor designs and four parameters will affect combustion efficiency. There will be many parameter combustions in the permutation of the operating condition. If all conditions were implemented, it would cost colossal time and expense. Therefore, this research employed the Kriging surrogate optimization model to predict the combustion efficiency tendency with fewer experimental runs. Utilizing the Kriging model can also obtain the sensitivity coefficient of the parameters and demonstrate the most influential parameter on combustion efficiency.

Paper ID: 309

Stage-V regulation compatible propane engine development for medium and large-sized construction machinery

Yongrae Kim (KIMM), Cheolwoong Park (Korea Institute of Machinery & Materials), Jisun Choi (Korea Institute of Machinery and Materials), Young Choi (Korea Institute of Machinery and Materials), Moonyong Jung (Blueplanet)

Due to the harmful emissions from the old diesel engines, it is needed to develop and spread a clean engine powertrain in a field of construction. So in this study, stage-V regulation compatible propane engine was developed for the medium and large-sized construction machinery. The fuel supply system was modified to deliver propane fuel and spark-ignition system was adopted to operate the gas fuel. Although the regulation is not fulfilled perfectly at this test, this engine can replace the old diesel engines without power reduction. More sophisticated control system will be introduced to this engine.

Paper ID: 310

The exergy analysis of methane, methanol, and hydrogen under constant-volume conditions

Jianan Wei (Tianjin University), Haifeng Liu (Tianjin University), Mingfa Yao (Tianjin University)

Low-carbon or carbon-free fuels like methane, methanol, and hydrogen have gained a lot of attention on their ability of CO2 reduction in Internal Combustion (IC) engines. In this context, improving thermal efficiency at reduced levels of emissions by adopting low-carbon fuels is meaningful in the current situation. However, the unconstrained combustion of exergy loss degrades the exergy-work transform in IC engines. The present study focuses on the exergy loss and the thermomechanical exergy of these low-carbon or carbon-free dual fuels blended with high reactive n-heptane as the diesel surrogate under engine-like conditions. Results reveal that hydrogen in blends shows more influence on exergy loss reduction than methanol and methane. Using low-carbon or carbon-free fuels in blends improves the thermomechanical exergy distribution at 1000-2000 K combustion range. In conclusion, the optimization of low-carbon fuels on exergy is mainly reflected in the low-temperature and rich mixture combustion conditions, thus, the use of low carbon fuels does improve exergy use in combustion processes where the mixture is not uniformly distributed.

Paper ID: 311

Experimental investigation on smoldering characteristics for sewage sludge

Xue Shen (Chongqing University of Science and Technology), Hui Yan (Chongqing University of Science and Technology), Jun Shi (Chongqing University of Science and Technology)

The disposal of sewage sludge has become a challenge in recent years. Smoldering combustion is a novel, low-energy, and promising new method for sewage sludge disposal. In this study, sawdust was used as auxiliary fuel to mix sewage sludge and sand to form a porous media fuel bed for smoldering combustion. The effects of key parameters such as moisture content, sand ratio, air flow rate and wood content amount on the sewage sludge smoldering characteristics, smoldering self-sustaining limits were explored to ensure stable operation in practical applications. The results showed that reducing the moisture content could improve the robustness of sewage sludge smoldering combustion and reduce the preheating time. Airflow rate and S/F ratios were the main factors controlling the peak temperature and smoldering velocity. The optimal S/F ratio was 3 kg/kg, when not only the smoldering velocity was maximum, but also sewage sludge with less sawdust added and higher moisture content could be treated.

Paper ID: 312

Performance of a micro-mixing nozzle under cO_2/N_2 dilution for CH_4-O_2 combustion

Xiangnan Chen (Beijing Institute of Technology), Kuanyu Wang (BIT), Xie Dingjiang (Beijing Institute of Technology), Yong Tang (Beijing Institute of Technology), Baolu Shi (Beijing Institute of Technology)

This work investigated micro-mixing combustion technologies based on cross-flow mixing of air and fuel to promote low-emission applications in future gas turbines. The major advantage of micro-mixing combustion is the inherent safety against flash-back and low nitrogen oxide (NOx) emissions due to the very short residence time of reactants in the reaction region. The purpose of this paper is to present the test results of a micro-mixing nozzle combustion diluted by carbon dioxide (CO_2) and nitrogen (N_2), and evaluate nozzle performance by focusing on flame structures. The results show that as the oxygen fraction decreases, the flame

can be divided into three regions, including the yellow region, the blue region and the blow-out region. The nozzle delivers stability and efficiency for operation in the blue region. The critical oxygen fraction where the flame changes from yellow to blue, and the blowing oxygen fraction where the flame changes from the blue region to blow off region, both increase with the flow rate of methane (CH_4). Compared to N_2 dilution, combustion diluted by CO_2 has the advantage of a shorter flame length and possible zero carbon-emission when combined with (Carbon Capture and Storage) CCS technologies.

Key words: micro-mixing combustion; CO_2 dilution; flame structure; oxygen fraction

Paper ID: 313

Effect of egr and hydrogen stratification on flame-wall interaction

Masato Sakurai (Tokyo Institute of Technology), Yamato Shiotsuki (Tokyo Institute of Technology), Masayasu Shimura(Tokyo Institute of Technology), Mamoru Tanahashi (Tokyo Institute of Technology)

Direct numerical simulations (DNS) have been performed for a laminar premixed flame propagating into an inert wall in a constant volume vessel with near-wall EGR and hydrogen stratification. The DNS results are analyzed to investigate the effects of near-wall EGR and hydrogen stratification on the wall heat flux and other parameters during flame-wall interaction. The DNS results have shown that the EGR stratification near the wall reduces the peak wall heat flux by approximately 90%. Also the effect of EGR is less pronounced for leaner conditions. Hydrogen-stratified methane combustion increased the wall heat flux in a short time, but the cumulative wall heat flux was similar to that of pure methane combustion.

Paper ID: 315

Effect of hydrogen in nitrous oxide on soot formation inverse diffusion flames: Adding on fuel stream

Eka Dwi Ariyanto (National Cheng-Kung University)

The Inverse Diffusion Flame (IDF) nitrous oxide–ethylene was studied with aiming of improving the understanding of soot formation. CH* and C_2* chemiluminescence was measured using spontaneous emission (chemiluminescence). Soot volume fractions were measured using the Laser-Induced Incandescence (LII) optical system. The main parameter is hydrogen addition in the fuel stream and points out the effect on soot formation. CH* represents the reaction zone and flame height. The results show that flame height will decrease when the hydrogen addition percentage increase. The flame structure is open tip can be seen in the CH* results. C_2* chemiluminescence showed the soot precursors and it is located in the carbonaceous zone. C_2* started above the reaction zone, and it will decrease when the hydrogen percentage increase. Soot volume fraction with LII systems changed similarly with CH* and C_2* chemiluminescence results. The results of soot volume fraction and chemiluminescence are closely related. The results show that the reduction in soot volume fraction is in line with the reduction of CH* and C_2* chemiluminescence. And it can be seen clearly in the flame luminosity that the high hydrogen concentration causes the blue region to increase and the brightness level to decrease.

Paper ID: 316

Jet-ignition of ammonia using hydrogen, *n*-heptane, and *iso*-octane as auxiliary fuels in a rapid compression machine

Zhang Ridong (Tsinghua University), Wei Liu (Tsinghua University), Qihang Zhang (Tsinghua University), Zhi Wang (Tsinghua University)

Ammonia is a promising fuel for internal combustion engines in the upcoming era where carbon-neutral is emphasized. Being hindered by strong combustion stiffness, ammonia is expected to gain easier ignition and faster combustion with the assistance of jet-ignition produced by highly-reactive fuels. This work investigates the jet-ignition combustion of stoichiometric ammonia mixture using various auxiliary fuels (H_2, NC_7H_{16}, and IC_8H_{18}) in a rapid compression machine. A single-hole jet chamber with hole diameter of 2 mm was adopted in experiments while the energy proportion of the auxiliary fuel to ammonia was all fixed at 5 %. Results show that the jet-ignition combustion duration shortens with increasing initial temperature. When using IC_8H_{18} as the auxiliary fuel, jet-ignition gains undesired combustion performance, which is reflected by the longer combustion duration when compared to other test fuels and some misfire cases at T_{EOC} = 690 K. H_2 serves as a promising auxiliary fuel for it helps achieve better ignition and combustion performance, which is attributed to H_2's higher reactivity and larger specific volume. Besides, auto-ignition and pressure oscillations were observed at T_{EOC} = 940 K, indicating the possibility of knock occurrence in internal combustion engines using ammonia as fuels at the current test condition.

Paper ID: 317

Effects of the DC electric field on a premixed flat flame formed in an impinging flow

Akira Shioyoke (Kyoto University), Yuki Fujita (Kyoto University), Hiroshi Kawanabe (Kyoto University), Jun Hayashi (Kyoto University)

To examine the possibility of controlling the combustion reaction intensity, an interaction between the electric field and the flame has been experimentally investigated. This study examined a flame shape deformation by applying a DC electric field in the impinging flow. From CH* chemiluminescence intensity, it was found that the flame position shifted in the direction opposite to the direction of the ionic wind by applying a positive voltage to the electrode placed on the impingement plate. It is considered that the laminar burning velocity is strongly reduced by flame deformation. Furthermore, the maximum intensity of CH* chemiluminescence and the width of the intensity distribution of CH* chemiluminescence were evaluated. It was shown that the intensity distribution of CH* chemiluminescence expanded toward the unburned side by applying a positive voltage. In addition, the results of spectrometry on the orange-red luminescence of burnt gas indicated that the luminescence of water vapor remarkably increased under the condition of applying a positive voltage.

Paper ID: 319

Evaluation on performance and emissions by commercial biodiesel fuels on a direct injection diesel engine

Mohammad Nor Khasbi Jarkoni (Universiti Malaysia Terengganu), Wan Nurdiyana Wan Mansor (Universiti Malaysia Terengganu)

Biodiesel emerged as one of the most promising energy solutions for reducing pollution and increasing

performance. Oxygenated alternative fuels are considered potential alternatives due to their efficient combustion and low emissions in engines. Combustion is a complicated process that greatly affects how well compression ignition (CI) engines work and how they emit gases. The commercial biodiesel blending fuel made up of 7% palm oil methyl ester (B7) and pure diesel (B0) was employed to investigate the effect on the performance and emissions characteristics. The ISO standard 8178: 4 Cycle D2 cycle, made up of five test runs at 2000 rpm. The result show brake-specific fuel consumption (BSFC) decreased and brake thermal efficiency (BTE) increased in B7. Engine emission characteristics such as hydrocarbon (HC), carbon dioxide (CO_2), and carbon monoxide (CO) were reduced significantly. However, nitrogen oxide (NO_x) was increased compared to pure diesel. Overall, the results discovered that biodiesel-diesel blending fuels could be a promising elective fuel with desirable properties, and better engine performance and emission characteristics.

Paper ID: 320

Two-dimensional simulation of turbulent soot flames using a two-equation model and various reaction mechanisms

Shion Ando (Kyushu University), So Shimamura (Kyushu University), Osamu Moriue (Kyushu University)

2D simulation of non-premixed turbulent combustion was performed using various reaction mechanisms to clarify the effect of reaction mechanisms on the accuracy of soot formation calculations. GRI-3.0, ABF (Appel-Bockhorn-Frenklach), DLR and KAUST were used as reaction models. Two-equation model was used as the soot formation model. The simulation results were verified with the Adelaide Jet EHN (Ethylene-Hydrogen-Nitrogen) flame. DLR and KAUST included hundreds of reactions, and the computational cost was heavy. Therefore, unimportant species were eliminated with DRG to reduce the computational cost. As a result, the effect of the reaction mechanism on the temperature distribution was small. On the other hand, the soot volume fraction was especially larger for GRI-3.0. This is probably because, in GRI-3.0, acetylene was not consumed for the formation of aromatics such as benzene. Instead, it was mainly consumed as a soot precursor. In addition, the soot volume fraction of reduced DLR was the smallest, which might be due to the accelerated oxidation of soot particles by O_2. It was suggested that the reaction mechanism has the influences on the mass fraction of species, which also has the effects on the soot formation simulations.

Paper ID: 321

Numerical investigation of the diluting effects of secondary air on the primary combustion zone of two-stage rich-lean ammonia gas turbine combustors

Ekenechukwu C Okafor (Kyushu University), Hirofumi Yamashita (Tohoku University), Osamu Kurata (National Institute of Advanced Industrial Science and Technology), Takahiro Inoue (National Institute of Advanced Industrial Science and Technology), Taku Tsujimura (National Institute of Advanced Industrial Science and Technology, AIST), Norihiko Iki (National Institute of Advanced Industrial Science and Technology), Akihiro Hayakawa (Tohoku University), Shintaro Ito (IHI Corporation), Masahiro Uchida (IHI Corporation), Hideaki Kobayashi (Tohoku University)

Two-stage rich-lean combustion has been demonstrated to be effective for the control of emissions from ammonia (NH_3) combustion. However, studies in gas turbine combustors suggest the possibility of an uncontrolled dilution of the primary zone (PZ) by the injected secondary air, which may limit the potentials

of two-stage rich-lean combustion and impair the stability of NH_3 flames. In this study, large eddy simulations of flows in models of two-stage gas turbine combustors were conducted to study PZ dilution and its effects on ammonia-methane-air combustion and emissions control. It was found that the PZ could be diluted by a large portion of the secondary air, and this is promoted by an increase in the secondary air flow rate and may encourage NOx emission due to non-uniformity of the mixture in the PZ. By controlling the flow of secondary air towards the PZ, a more uniform equivalence ratio in the PZ and hence lower overall NOx emission was achieved. However, mitigation of PZ dilution in this study promoted NO, NO_2 and N_2O production in the secondary zone.

Paper ID: 322

Stochastic modelling of premixed combustion in microchannels

Matthew M Kratzer (University of Queensland), Suresh Bhatia (University of Queensland), Alex Klimenko (The University of Queensland)

This work investigates a stochastic method of modelling reacting flow in smooth channels of the mesoscale. By investigating the Fokker-Planck equation governing flow through a 1D channel with the inclusions of particle-particle collisions, particle-particle reactions and particle-wall collisions, the effect of wall roughness and fluid rarefication on mixture mass fraction is analysed.

Paper ID: 323

Effect of impingement position on the structure of non-premixed hydrogen-oxygen impinged jet flames

Hazim Shehab (National Institute of Advanced Industrial Science and Technology), Yong Fan (National Institute of Advanced Industrial Science and Technology), Norihiko Iki (National Institute of Advanced Industrial Science and Technology), Osamu Kurata (National Institute of Advanced Industrial Science and Technology), Taku Tsujimura (National Institute of Advanced Industrial Science and Technology), Hirohide Furutani (National Institute of Advanced Industrial Science and Technology)

This study investigated the structure of non-premixed hydrogen-oxygen flames using single-pair versions of the micro-impinged jet array (MIJA) burner. As two oxygen jets impinge at an acute angle on the hydrogen jet, the burner facilitates a forced mixing of hydrogen and oxygen at the impingement point, which improves flame holding. We examined the effect of impingement position on the flame structure with two different nozzles. Short laminar flames were observed in rich conditions, while highly turbulent V-shaped flames were observed in lean conditions. In the stoichiometric condition, a turbulent V-shaped flame was observed for the nozzle with a further impingement position but not for the other nozzle with a closer impingement position. The oxygen-to-hydrogen jet momentum ratio (M_{O2}/M_{H2}) at the impingement position was evaluated using analytical analysis for freely propagating jets. As gas jets traveled downstream, they diverged, resulting in less effective momentum flux at the impingement position. However, the hydrogen jet retained more momentum flux than the oxygen jets due to shorter travel distances. Thus, M_{O2}/M_{H2} became larger as the impingement position moved further downstream. Furthermore, a critical M_{O2}/M_{H2} was reached at a further impingement position, yielding the formation of the V-shaped flame.

Paper ID: 326

A numerical study on the determination of laminar flame speed using contracting-nozzle-generated counterflow flame configuration

Wenfeng Shen (JiMei University), Zhijie Chen (JiMei University)

The counterflow flame configuration is widely used to determine the laminar flame speed (S_u^0), which is extrapolated from experimentally measured reference flame speeds ($S_{u,ref}$) at various stretch rates (k). The relation of Su,ref and k is usually theoretically and numerically analyzed with the assumptions of a quasi-one-dimensional system along the centerline of the counterflow configuration. A two-dimension simulation of a contracting-nozzle-generated counterflow methane premixed flame configuration was carried out with finite rate chemistry in this study. 1D simulations with plug-flow and potential-flow boundary conditions were also conducted and the simulation data was compared to the 2D simulation data to quantify the errors raised by quasi-1D assumptions. The results show that the extrapolated error could be reduced to under-measurement uncertainty when the axial velocity gradient at the burner exit is used as a boundary condition in the 1D plug-flow model. The extrapolation using the potential flow condition also performs well, which provides an alternative and convenient method for calculating extrapolation curves.

Paper ID: 327

Effects of capacity and charge of lithium ion battery on fire characteristics

Sin Woo Kim (Pukyong National University), Eui Ju Lee (Pukyong National University)

The effects of capacity and the state-of-charge (SOC) of a lithium ion battery on fire characteristics were investigated using a cone calorimeter and a smoke density chamber. The fire characteristics featured two combustion stages, with the first and second characterized by a diffusion flame and a partially premixed flame, respectively. Although the overall heat release rate (HRR) characteristics were affected by both the battery capacity and the SOC, the capacity affected the HRR of the secondary stage less than did the SOC. A stronger explosion and greater emissions of CO and smoke at a higher SOC support the fact that partial premixing of the second combustion stage is characterized by self-evolution of oxygen. We introduced and confirmed a comprehensive parameter to indicate the degree of combustion and the risk of battery fires.

Paper ID: 328

Analysis of the borderline of no-ignition and mild combustion regimes of methane, propane, and syngas fuels based on ignition delay time

Srinivasarao Muddada (IIT Kharagpur), V. Mahendra Reddy (Indian Institute of Technology Kharagpur)

The ignition delay time (IDT) is one of the significant parameters to describe flame behavior. The regime diagrams of the methane, propane and syngas fuels are collected to investigate the IDTs in different regimes (no-combustion, borderline (between MILD and no-combustion), MILD, and HITAC). In each fuel combustion regime diagram, a few points from different regimes are extracted for the analysis of IDTs. The IDTs are calculated using numerical simulations for all the collected data points. The same range of IDT magnitude is observed for the borderline points. However, the magnitude varied based on the fuel type and composition. The IDTs for the borderline data points are also calculated using available IDT correlations in the literature. It is observed that the available correlations are not predicted well for the borderline data points.

Hence, this study proposes a correlation for calculating IDTs at the considered borderline for methane, propane, and syngas. Furthermore, the proposed correlation is well validated with available border data points of methane-stabilized MILD combustion. In addition, a methane-hydrogen combustion regime diagram is constructed, and IDTs of borderline data points are compared with the proposed correlation. The maximum error between the proposed correlation and numerical simulations is within 7 %.

Paper ID: 329

Study on the influence of the external acoustic forcing on lean blow-off limit in a confined premixed dme/air swirling flame

Chen Fu (Shanghai Jiao Tong University), Meng Wang (Shanghai Jiao Tong University), Xiaoyang Wang (Shanghai Jiao Tong University), Kunpeng Liu (Shanghai Jiao Tong University), Yifeng Jiang (Shanghai Jiao Tong University), Yi Gao (Shanghai Jiao Tong University)

The present work aims to understand how external excitation influences the lean blow-off limit. A confined premixed DME/air swirling flame in a cylindrical quartz enclosure stabilized on an axisymmetric bluff body has been investigated experimentally. The flames forced at two frequencies of external acoustic excitation, 10 Hz and 400 Hz, are compared with varying excitation amplitude. The blow-off characteristics are recorded with simultaneous PIV and OH* chemiluminescence. It is found that the flame response to the velocity fluctuation is different at two frequencies. The flame height and global heat release vary when excited at 10 Hz, and the flame root is twisted with constant flame height and global heat release when excited at 400 Hz. At the same bulk velocity, the flame excited at 10 Hz can survive a higher forcing amplitude than that of 400 Hz. It is probably due to the flame heat release varying in phase with the outlet velocity at 10 Hz, but it keeps stable at 400 Hz.

Paper ID: 330

Flow field characterization of a flickering buoyant jet diffusion flame

Haodong Zhang (Shanghai Jiao Tong University), Yifan Yang (Shanghai Jiao Tong University), Linye Li (Shanghai Jiao Tong University), Mingming Gu (Shanghai Jiao Tong University), Xi Xia (Shanghai Jiao Tong University)

The flickering behavior of diffusion flames reflects a classical flame instability problem. This paper presents an experimental study on the flickering behavior of buoyant jet diffusion flame originating from a round nozzle. Based on a simultaneous high-speed particle image velocimetry (PIV)/flame brightness measurement system, the flow field inside and outside the flame is acquired together with the synchronous flame sheet. Furthermore, a detailed vortex-dynamical analysis of the flow and flame structures is performed to verify the outer vortex ring (OVR) mechanism contributing to the flickering behavior. Results confirm that the periodical growth and shedding of OVRs cause the stretching, neck-in, and pinch-off of the flame sheet. The instability onset is characterized by the generation of a new vortex core in the outer shear layer (OSL) near the flame root, the development process of which can be divided into three stages based on the evolutions of the vorticity and the vortex core location.

Paper ID: 331

Computational modeling and simulation of ignition and combustion of nitromethane

SK Hossen Ali (Indian Institute of Technology Gandhinagar), Dilip Sundaram (Indian Institute of Technology Gandhinagar)

A computational analysis of ignition and combustion of gas-phase and liquid nitromethane is conducted. Chemical equilibrium analysis is first conducted to compute specific impulse of nitromethane with and without metal additives and comparison is drawn with conventional liquid mono- and bi-propellants. A unified theoretical and computational framework is developed to predict ignition and combustion behavior of gas-phase and liquid nitromethane. The model treats all important underlying physicochemical phenomena such as heat and mass transfer, fluid flow, chemical kinetics, and phase change within the CFD framework and an effort is made to mimic the experimental conditions. The framework is first validated by simulating ignition and combustion behaviors of premixed H_2-air and CH_4-air mixtures. The validated framework is then used to study ignition and combustion of nitromethane. Reactor flow simulations are first conducted to study the effects of temperature on ignition delay of pure gas-phase nitromethane. Flame speeds are computed using propagation method for different pressures in order to understand the effect of pressure on the flame speed of gas-phase nitromethane. Further, comparison is drawn with the experimental liquid nitromethane regression rates. Finally, regression rates of liquid nitromethane are computed using the developed framework and the predictions are compared with the experimental data.

Paper ID: 332

Experimental and theoretical study on the ignition process of boron particle

Ying Feng (Beijing Institute of Technology), Yong Tang (Beijing Institute of Technology), Wei Dong (Beijing Institute of Technology), Xie Dingjiang (Beijing Institute of Technology), Majie Zhao (Beijing Institute of Technology), Baolu Shi (Beijing Institute of Technology)

The ignition process of boron particles is a crucial stage for its practical application in engines, however, this process is very complicated. To explore the ignition characteristics of fine amorphous boron particles, an experimental apparatus using a Hencken multi-diffusion flat flame burner was utilized to construct a high-temperature oxygen-containing exhaust and measure the ignition time of small sized boron particles. The results indicate that the ignition time increases with decreasing ambient temperature and oxide layer thickness. An ignition model consisting of two evaporation processes and three heterogeneous reactions was established to predict the change of oxide thickness and ignition time. It has been demonstrated that the proposed model presented good agreement with the measured ignition time.

Paper ID: 333

Multi-species laser sensing in shock tube kinetics using CEAS and DDAE

Mhanna Mhanna (KAUST), Mohamed Sy (KAUST), Ali Abualsaud (KAUST), Jiabiao Zou (KAUST), Ali Elkhazraji (KAUST), Aamir Farooq (KAUST)

Chemical kinetic experiments of fuel oxidation/pyrolysis are quite complicated with a multitude of species being formed and consumed. It is desirable to have a diagnostic strategy that can detect several species simultaneously with high sensitivity, selectivity and fast time response. In this work, a mid-infrared laser

sensor is presented for selective and simultaneous multi-species detection in high-temperature shock-tube experiments. Time-histories of major products of ethanol pyrolysis are measured behind reflected shock waves at T = 1000 – 1500 K and P = 1 atm. The sensor is based on a distributed feedback inter-band cascade laser emitting near 3.3 μm. Wavelength tuning over 3038.6 – 3039.8 cm-1 and denoising models based on deep denoising auto-encoders (DDAE) are employed to differentiate the broadband absorbance spectra of evolving species. The models are able to clean noisy absorbance spectra and split these in to contributions from reference species by multidimensional linear regression (MLR). Off-axis cavity enhanced absorption spectroscopy (CEAS) is also implemented to improve sensitivity to weak absorbers by amplifying effective laser interaction length. The minimum detection limit of the sensor is 2.9 – 7.2 ppm of target species in argon bath gas for a 14.22-cm apparent pathlength.

Paper ID: 334

Combustion modeling of multi-grains in closed bomb using volume of fluid and fluid structure interaction methods

Jonggeun Park (Korea Aerospace University), Jeongseok Kang (Korea Aerospace University), Hong-Gye Sung (Korea Aerospace University)

A precise numerical study on a closed bomb combustion has been conducted to investigate the combustion characteristics of multi-grains and the movement of grains using the Volume of Fluid (VOF) method and Fluid Structure Interaction (FSI) method. The fluid structure interaction (FSI) method is implemented to analyze the interaction between gas and solid at the same time. The Eulerian analysis and Lagrangian analysis methods are applied for the gas and grain combustion and for the grain movement, respectively. The forces acting on the grain consist of pressure at the burning surface and gravity. The VOF method is used to simulate the burning distance and the movement of the grains. The combustion analysis is performed for 100 grains and compared with the experiments.

Paper ID: 336

PIV measurement and numerical simulation of flow field in a novel burner with a cap

Ching-Huan Tseng (National Taiwan University), Pei-Hsun Huang (National Taiwan University), Kuo-Long Pan (National Taiwan University)

This work investigates the burning of a new device that has a recirculation zone of a bluff-body and an inner space of a cap structure for creation of premixing fuel and air. Four basic flame modes, defined as jet-like flame, transition flame, premixed-like recirculated flame and premixed-like jet flame, were considered. They corresponded to the settings of the co-flow air velocity being at 0.38, 1.5, 2.65, 3.75 m/s, respectively, when the velocity of central fuel was fixed at 1.2 m/s. Also, the particle image velocimetry (PIV) was used to analyze both the inner and outer flow fields of the cap burner to obtain an average streamlined diagram, as well as the profiles of flow velocity and vorticity. By means of numerical simulations of the cap burner and a disc burner, the heat release and the temperature distributions could be analyzed and compared. The computational results were compared with the experiments of the disc and the cap burners, so as to help further development of the combustor.

Paper ID: 337

Profiles of flow parameters of supercritical n-heptane flows inside a convergent nozzle

Guigui Liu (Beihang University), Yuzhen Lin (Beihang University), Xin Xue (Beihang University), Xin Hui (Beihang University), Chih-Jen Sung (University of Connecticut)

The in-nozzle flow characteristics of n-heptane (C7) at a supercritical pressure injected into an atmospheric environment were investigated experimentally, with special emphasis on the effects of fuel injection temperature on the phase transition and profiles of flow parameters. The injection pressure was fixed at a supercritical value and the injection temperature was varied from supercritical to subcritical value. It was found that the measured pressure near the nozzle exit first increases and then decreases with the decrease of injection temperature. The fuel phase transition during the expansion process was analyzed based on a reduced entropy-pressure phase diagram and a one-dimensional estimation. Results showed that C7 flows originating from different phase state regions can experience different phase transition during the expansion process. The profiles of the fuel temperature drop and density drop along the axis of the nozzle were further evaluated, it was discovered that the variation trend of these two parameters with the injection temperature is reversed under the high injection condition and low injection condition. Further analysis suggested that the unique evolution of specific heat ratio and compressibility factor along the injection path, caused by distinct phase transition during the fuel expansion, have a great impact on the profiles of flow parameters.

Paper ID: 338

Influence of wall roughness size and fuel non-equidiffusivity on laminar boundary layer flashback

Louis Benteux (THU), Damir Valiev (THU)

Multiple previous studies focused on the impact of the wall roughness on flow characteristics, but few considered the effect of wall roughness on a boundary layer flame flashback. In the present study, laminar boundary layer flashback (BLF) is simulated in channels with wall roughness using a finite volume solver. The BLF process is modeled by simulating the interaction of a laminar premixed flame with a parabolic shear flow in a planar channel. Triangular roughness elements are used, and the effects of the geometry of the elements on the BLF are studied. The simulations confirm that wall roughness may attenuate the flashback tendency due to the enhanced heat loss to the wall boundary. It is shown that the critical velocity gradient depends on the roughness base size non-monotonically. It is also confirmed that an increase in the Lewis number decreases the propensity of BLF.

Paper ID: 339

Investigation of non-reaction field turbulent flow in hybrid fractal grid

JungHyun Kim (Suncheon University), Keeman Lee (Suncheon University)

This study experimentally investigated the non-reaction field flow characteristics by the shape parameters of the hybrid fractal turbulence generator, which improved the conventional circular fractal turbulence generator. The circular hybrid fractal turbulence generator was designed by combining the cross-type and square-type used in previous studies. A V-shaped flame using a flame stabilization rod is used to evaluate a circular hybrid fractal turbulence generator. The mean velocity and velocity fluctuation of hot-wire anemoentry in axial and radial directions were investigated. As a result, it was confirmed that the turbulence intensity of the z-axis

increased and inhomogeneity was improved with the change in the blockage rate and Rt of the hybrid fractal turbulence generator.

Paper ID: 342

A study on the characteristics of the low swirl combustion generated from a hybrid fractal grid

Geonryul Lee (Sunchon National University), Keeman Lee (Sunchon National University)

This study investigated the low-swirl turbulent flow characteristics combined with the hybrid fractal grid, and studied the correlation between the turbulence intensity of the combustion reaction field and structural variables of the grid. The turbulence intensity before the nozzle outlet showed the characteristics of the cross grid. Turbulence intensity increased in the descending order of RRBT, and the maximum point was located with order of RRBT. The combustion reaction field was characterized by variable(x*)containing structural information of the grid, and the correlation between the characterized flow and $I^2/I^2_{peak}$was identified. The coefficient of determination (R^2) differed with the number of iteration and shape of the grid, and at I3, it was the highest in x_s^* including the square grid variable.

Paper ID: 345

Improving chemical mechanism for NH_3/H_2 combustion and adaptation of artificial neural network (ANN) for acceleration of the simulation

Serang Kwon (Korea University), Seongkyun Im (Korea University)

Ammonia is a carbon-free fuel. However, ammonia combustion can emit NOx and unburned ammonia, which are toxic to public health. Therefore, predicting chemical products of ammonia combustion by simulation is required. Accuracy of the simulation is enhanced by adopting a chemical mechanism with lower error from experiments. Furthermore, the simulation should be accelerated, especially if it is multidimensional. Thus, this paper investigated improving the mechanism of NH_3/H_2 combustion and an artificial neural network (ANN) to accelerate the simulation by substituting the solver. Improving the chemical mechanism was performed by finding a combination of the reactions that demonstrated minimum error with experimental datasets. Significant number of combinations of reactions were created from four existing chemical mechanisms by Monte Carlo method. A combination displaying smaller error with experimental data than the existing mechanisms was selected as an improved chemical mechanism. Employing the mechanism, a dataset for the ANN was created from calculation of a nondimensional isobaric adiabatic reactor with varied initial conditions. The ANN showed better prediction accuracy at steady time, but lower accuracy at earlier transient state. The accuracy could be increased by size of the timesteps. Further, recurrent neural network would be considered to increase the prediction accuracy of ANN.

Paper ID: 347

A multi stage kinetic reaction optimization strategy applied to n-heptane combustion mechanism

Krunal R Panchal (Indian Institute of Technology), Vaisakh Vasudaven (Lennox India Technology Center), Krithika Narayanaswamy (Indian Institute of Technology)

In the current work, a novel multi-stage optimization strategy is proposed. The aim of the work is to reduce the cost of optimization of reaction mechanism. The strategy relies on the fact that the reaction pathways

important at high and low temperature are different. Therefore, the dominant reactions at the high and low temperatures are optimized in separate stages in this approach. The idea is demonstrated using a three-stage optimization of a n-heptane mechanism as a case study. Experimental targets for n-heptane were chosen at P:13.5 – 42 atm, T: 665 – 1331 K and equivalence ratio of 1 – 2. An approximation technique, namely polynomial response surface (PRS), is used to eliminate the need for a differential equation solver within the optimization framework. Genetic Algorithm (GA) is used to carry out the optimization study. It is found that the multistage optimization strategy reduces the optimization cost by ~45 % compared to classical single stage optimization technique for the case-study considered.

Paper ID: 349

Experimental investigation of thermal behaviors of the components of high nickel lithium-ion batteries under various states of charge

Ayushi Mehrotra (Seoul National University), Juyoung Oh (Seoul National Univ Korea), Yejun Lee (Seoul National University), Jack J. Yoh (Seoul National Univ Korea)

The main safety issue that hinders the utilization of Lithium –ion batteries (LIBs) on a large scale pertains to the thermal runaway (TR) phenomenon, which is one of the main causes of the failure of the lithium-ion battery. In the present study, two high-Nickel Lithium-ion battery samples: NCA 88 and NCA 91 Nickel Cobalt Aluminum: $Li[Ni_{1-x-y}\ Co_x\ Al_y]O_2$ with 88% and 91% Nickel content (%wt) as cathode and Silicon-Carbon Nanocomposite (SCN) as anode at five different states of charge (SOCs) are examined. The thermal analysis was performed using the Differential Scanning Calorimetry (DSC) technique. It is observed that increase in Nickel content adversely affects the thermal stability of the battery. This is due to the increase in the evolved oxygen with relation to the Nickel content, which aids in triggering the TR phenomenon. On increasing the Nickel content, the onset temperature of the TR phenomenon decreases. It was also observed that for SOCs greater than 50%, the probability for thermal runaway increases and the triggering reaction is identified to be the decomposition of the Solid Electrolyte Interphase (SEI) layer. It was also observed that the probability of the thermal runaway phenomenon is the greatest for SOCs ranging from 75% to 100% for both battery samples.

Keywords: High-nickel Lithium-ion batteries; Thermal Runaway; Thermal analysis; Differential Scanning Calorimetry

Paper ID: 351

Effects of oxygen concentration of oxygen enriched $CH_4/O_2/N_2$ flames in temperature measurements using LITGS at 1.0 Mpa

Hiromi Kondo (Tohoku University), Yuta Mizuno (Tohoku University), Taku Kudo (Tohoku University), Akihiro Hayakawa (Tohoku University)

Quantitative measurement of temperature using Laser Induced Thermal Grating Spectroscopy (LITGS) for oxygen enriched $CH_4/O_2/N_2$ premixed flames at 1.0 MPa were carried out. The effects of product gas composition and density on the measurement accuracy of temperature and the grating formation in LITGS were investigated. The oxygen ratios in $O_2 + N_2$ mixture were varied from 0.21 to 0.55. In addition, the grating spacing was changed by adjustment of alignment, and the effects of grating spacing on the temperature measurements were experimentally investigated. The results showed that the differences between derived

temperatures from LITGS signals and those from numerical simulations were increased with an increase in the oxygen ratio. It was caused by a decrease in the density and the change in mole fraction of the quenching species at the measurement point, particularly H_2O. It was also shown that even under oxygen enriched cases, the measurement accuracy of temperature can be improved by increasing the grating spacing because the thermal grating formation approaches to the promising grating generation. It was also discussed from the standpoint of the signal contrast.

Paper ID: 352

On the autoxidation of limonene under cool flame conditions: formation of oxygenated and aromatic products

Zahraa Dbouk (Centre National de la Recherche Scientifique), Nesrine Belhadj (Centre National de la Recherche Scientifique), Maxence Lailliau (Centre National de la Recherche Scientifique), Roland Benoit (Centre National de la Recherche Scientifique), Philippe Dagaut (Centre National de la Recherche Scientifique)

The oxidation of limonene-O_2-N_2 mixtures and 1-methyl-cyclohexene-O_2-N_2 mixtures was conducted in a jet-stirred reactor (JSR) in the cool flame regime, fuel-lean conditions, and atmospheric pressure. Samples of the reacting mixtures were collected and analyzed by (i) on-line Fourier transform infrared spectroscopy, (ii) gas chromatography-mass spectrometry (GC-MS), and (iii) high resolution mass spectrometry after direct injection or chromatographic separation using reversed-phase ultra-high-performance liquid chromatography and +/– heated electrospray ionization and +/– atmospheric pressure chemical ionization. H/D exchange using deuterated water and reaction with 2,4-dinitrophenylhydrazine were performed to probe the presence of OH, OOH, and C=O groups in the products, respectively. A broad range of oxidation products ranging from final products to highly oxygenated products with five and more O-atoms, was detected. Besides, a range of aromatic and poly-unsaturated products were also detected. A range of tools were used to characterize and rationalize the data: Van Krevelen plots, computation of the degree of unsaturation in products

Paper ID: 353

Numerical study of multiband-multiline tomographic absorption spectroscopy for flame measurements

Tengfei Jiao (Sichuan University), Kin-Pang Cheong (Sichuan University), Wenju Hu (Sichuan University), Yushuai Liu (Chinese Academy of Sciences), Liuhao Ma (Wuhan University of Technology)

A novel thermometry method, multiband-multiline thermometry (MMT), was proposed and numerically validated in the present work. The method utilizes information of multi transitions in separate spectral windows (e.g, rotational-vibration bands) which have respective sensitivities for different ranges of temperature. Compared with the conventional method, the two-line thermometry (TLT), MMT compensates the disadvantage of limited detection range of temperature. Three typical spectral segments are chosen in this work for comparisons because these segments contain the transitions which are commonly utilized in TLT by other researchers. Numerical results show that MMT combining with tomographic algorithm effectively solves the region in high-temperature gradient of the flame. For axisymmetric and non-axisymmetric flames,

the MMT method combining respectively with Abel inversion and algebraic reconstruction technique (ART) effectively reconstructs the complete temperature and species concentration profiles with superior accuracy and robustness. The present numerical study demonstrated that MMT shows great potential in detecting the region with large temperature gradient which varies from indoor temperature to high temperature of combustion in the cost of adding only one or a few tunable laser sources.

Paper ID: 354

Oxygen and pressure effects on the ignition of polymer-insulated wire with short-term excess current in microgravity: a numerical study

Feng Guo (Hokkaido University), Nozomu Hashimoto (Hokkaido University), Osamu Fujita (Hokkaido University)

Non-standard atmospheric conditions in spacecraft may affect the flammability limits of materials. The ignition characteristics of polymer-insulated wires with a short-term excess current in microgravity under different atmospheric conditions were investigated through 2-dimensional numerical simulations. Three sets of atmospheric conditions were performed under different enriched oxygen concentrations at 1 atm, varied sub-atmospheric pressures of air, and constant partial pressure of oxygen at reduced total pressures. The ignition maps in terms of ignition energy and ignition delay time were investigated. By analyzing the ignition positions, the spontaneous ignition mode can be found in most scenarios where minimum ignition energy (MIE) was applied. The MIE value of the spontaneous ignition mode is almost independent of the time the electric current is applied. The MIEs decrease with enriched oxygen but increase with reduced total pressure. Under sub-atmospheric air pressure, a non-ignition regime with higher applied energy was found due to the termination of pyrolysis, which separates the wire-assisted ignition mode from the ignition map. The increased MIEs under reduced total pressure with constant oxygen partial pressure implied the importance of diffusion of pyrolysis gas from the wire insulation.

Paper ID: 355

Development and validation of compact kinetic model for high temperature oxidation of 3-hexene

Lalit Y Attarde (Indian Institute of Technology), Krithika Narayanaswamy (Indian Institute of Technology)

Alkenes are an essential component in transportation fuel composition and also appears as major intermediates in alkane chemistry. Alkene with double bond in the middle of the molecule is particularly interesting to study, as this can represent the long chain unsaturated methyl ester, with double bond in the middle, and serve as surrogate for biodiesels. Therefore, studying and depicting accurate chemical kinetic behavior of alkenes is necessary. In this study, the trans-3-hexene mechanism is developed for the high-temperature range of 1000K-1600K. The base chemistry of the NUIG1.3 comprehensive mechanism is included in the present mechanism. Various revisions are incorporated based on the literature survey and the latest theoretical reaction rates. The 3-hexene mechanism produces a good agreement with ignition delay times measured in shock tube experiments for different equivalence ratios and pressures. Laminar flame speed is also well-validated with experimental data for atmospheric conditions. This work will be carried further to develop low-temperature chemistry for trans-3-hexene in the future.

Paper ID: 356

A comparative study of reaction mechanisms towards predicting NOx in methane/hydrogen premixed flames

Md Adil (Indian Institute of Technology Madras), Krithika Narayanaswamy (Indian Institute of Technology Madras)

Mitigating NO_x emissions during lean combustion of methane and hydrogen blends in industrial gas turbines is quintessential. To predict NO_x precisely, accurate kinetics are crucial. As a first step, this work assesses different kinetic mechanisms in the literature with regard to their ability to predict NO in premixed flames. The present study investigates four kinetic mechanisms, namely FFCM mech, SanDiego mech, Hou et al. mech, and reduced Aramco mech mechanisms, the reduced Aramco mech mechanism is selected as having the best base chemistry among the four mechanisms based on the flame speed and ignition delay validation tests. In addition, two nitrogen chemistries, one from the Glarborg et al. and the other from the Hou et al. mech, are also studied. It is found that the Nitrogen chemistry from Glarborg is better at predicting the NO concentrations in the heat flux burner.

Paper ID: 357

Large eddy simulation of a turbulent dimethyl ether jet flame with direct moment closure model

Runzhi Liu (Zhejiang University), Kun Luo (Zhejiang University), Tai Jin (Zhejiang University), Jianren Fan (Zhejiang University)

Recently, a novel direct moment closure (DMC) model has been developed and systematically validated to account for the turbulence-chemistry interactions. In the present study, the DMC model is further adopted to simulate the experimental DME piloted jet flame in the framework of large eddy simulation, with a detailed DME oxidization mechanism of 55 species and 290 reactions. The numerical results are comprehensively validated against the experimental data of the flame. The predictions of the LES-DMC present good agreement with the experiment data for the radial distribution of the mean and fluctuations of axial velocity, temperature, mixture fraction and species. Besides, the conditional mean value of temperature and species mole fraction for the LES-DMC modeling is also consistent with the experiment data. It is demonstrated that the direct moment closure model can be applied to the simulation of turbulent flames with complex reaction mechanisms and exhibit high accuracy in the context of the large eddy simulation.

Paper ID: 358

Low-pressure ignition and combustion characteristics of a dual-mode ionic liquid propellant in a catalyst bed reactor

Zun Wang (Tsinghua University), Jie Fang (Beijing Institute of Control Engineering), Shaolong Li (Tsinghua University), Zhaopu Yao (Beijing Institute of Control Engineering), Shuiqing Li (Tsinghua University)

This paper experimentally investigates the ignition and combustion characteristics of a kind of mixed and energetic ionic liquids in a catalytic bed reactor. Firstly, the ignition performances at various preheating temperatures and pressures are examined. Then, the combustion process after the sustainable ignition is optically observed. It is found that the local zone with a high temperature accelerates the sintering of the catalyst. Finally, the change in catalyst structure after the catalytic combustion is tested by chemisorption

methods (BET) and transmission electron microscopy (TEM). The specific surface area and pore volume of the catalyst decreases whereas the pore diameter increases. It suggests the deactivation of the catalyst. Finally, such deactivation might be mainly attributed to the sintering, inferred from the decreased dispersion of iridium(Ir) crystals on the catalyst.

Paper ID: 359

An extend measurement of auto-ignition and kinetic model assessment for RP-3 aviation kerosene

Congjie Hong (Xi'an Jiao Tong University), Wuchuan Sun (Xi'an Jiao Tong University), Wenlin Huang (Xi'an Jiao Tong University), Wu Honghuan (Xi'an Jiao Tong University), Zuohua Huang (Xi'an Jiao Tong University), Yingjia Zhang (Xi'an Jiao Tong University)

In *this study*, a new injection experiment strategy in shock tube experiments was proposed and systematically validated. Results showed that the injection strategy reproduces well the experimental results obtained by traditional premixed method, and expands the range of auto-ignition experiments for low saturated vapor pressure fuels. By using the injection strategy, ignition delay times of RP-3 aviation kerosene/air mixtures were measured under a wide range of conditions, covering temperature of 650-1300 K, pressure of 7.5-30 atm and equivalence ratio of 0.5-1.5. Performance of existing chemical kinetic models of RP-3 surrogate fuel was evaluated using the ignition delay data measured in *this study*. Comparison indicated that the existing models can not capture the auto-ignition characteristics of RP-3 under the entire test conditions, negative temperature coefficient regime in particular. With current tests, we provide a broader ignition delay data set which is valuable for design of engine combustor and verification of kinetic model of RP-3.

Paper ID: 360

Low to high temperature oxidation of *n*-dodecane/air mixtures

Congjie Hong (Xian Jiaotong University), Chunyu Wang (Xi'an Jiaotong University), Yilong Ao (Xi'an Jiaotong University), Wuchuan Sun (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University), Yingjia Zhang (Xi'an Jiaotong University)

N-dodecane is a typical surrogate fuel in kerosene and diesel. In this paper, the shock tube experiment of *n*-dodecane in a wide temperature range had been carried out, and compared with the prediction value of the latest n-dodecane model. The results showed that there was a large deviation between the predicted values of the model and the experimental results in the low temperature region. Theoretical analysis was carried out to solve this problem. It was found that the rate coefficients of $\dot{O}_2$QOOH isomerization reactions have a great impact on the prediction performance of the model in the low temperature region. How to accurately select or calculate the rate coefficients of $\dot{O}_2$QOOH isomerization reactions needs further in-depth research.

Paper ID: 361

On the stability of steady symmetric flames propagating from an open towards a closed end of a narrow channel

Chengxi Miao (Tsinghua University), Damir Valiev (Tsinghua University)

Dynamics of a premixed flame propagating from an open to a closed end of a narrow channel with adiabatic nonslip walls is studied numerically. The main focus of the present study is on the symmetry breaking process

of flame shape. It is shown that, for certain channel widths, an initially symmetric concave steady flame may acquire a non-symmetric shape upon imposing a small perturbation. For wide enough channels, the amplitude of the perturbation grows exponentially until the non-symmetric flame is formed after sufficiently long time. It is shown that the flame instability is of hydrodynamic nature: the flow is generated in the unburnt fuel due to the thermal gas expansion, with the wall-normal component of the velocity playing a vital role in symmetry breaking. The instability growth rates are quantified for a range of channel widths and gas expansion ratios. It is shown that the instability growth rate increases with the thermal gas expansion.

Paper ID: 362

Volume-of-fluid simulations of spray injection in a coaxial air-blast atomizer

Po-Han Chen (KAUST), Alberto Ceschin (KAUST), Francisco Hernandez Pérez (KAUST), Hong G Im (KAUST)

Air-blast atomizers are commonly used in gas turbines, and its atomization characteristics has a significant effect on combustion efficiency and pollutant formation. In the present study, high-fidelity simulation of the water injection in a coaxial air-blast atomizer is undertaken and validated with experimental data. To precisely determine the interface between two phases, two-phase flows were modelled using the volume-of-fluid (VOF) formation combined with the *isoAdvector* and *PLIC-RDF* methods for the interface description. An incompressible turbulent flow is solved with the large eddy simulation (LES) approach. Droplets that are smaller than computational cells are substituted by Lagrangian particles in the simulation process. The simulation results of the air inlet of a coaxial air-blast atomizer are found to agree with the experimental data.

Paper ID: 363

Detection of extreme events in hydrogen combustion relevant to reheat burners

Dibyajyoti Nayak (Indian Institute of Science), Konduri Aditya (Indian Institute of Science)

Hydrogen's highly reactive and diffusive nature poses severe challenges, such as flashbacks and flame instabilities, in firing gas turbine engines toward decarbonization. The flame instabilities that appear due to intermittent pressure and temperature fluctuations compromise the engine's performance. In this study, we develop a statistical learning-based tool that leverages the properties of principal vectors obtained from the singular value decomposition (SVD) of the co-kurtosis tensor of engine data to detect the early inception of spontaneous ignition kernels that appear due to temperature fluctuations in lean premixed hydrogen combustion at vitiated conditions. The datasets used comprise species mass fractions, temperature, pressure, and velocities, obtained from numerical simulations at different operating pressures. We observe that the inception of an ignition kernel can be characterized based on the principal values and vectors, using which a detection algorithm is developed. The accuracy of the detection model is assessed.

Paper ID: 364

A study on the extinction behavior in interactive NH_3/CH_4 premixed flames

Jin Eunseo (Center for Aerospace Engineering Research), Keeman Lee (Sunchon National University)

Experiment and numerical data were compared through a counterflow burner to understand the interaction of the ammonia/methane mixture. To use an accurate numerical mechanism, the extinction boundary of the flame

at strain rate (a_g) was verified, and the Okafor's mechanism showed satisfactory experimental results. The previously verified mechanism was used to show the stability map of the flame in the ammonia/methane mixture, and the extinction behavior of the flame could be explained through the volume-based effective Lewis number ($Le_{v,\,eff}$) and the insufficient reactant Lewis number (Le_D). The chemical interaction between flames in the downstream was investigated through major species, key radicals and chemical reaction pathways in the flame of the extinction condition. It was confirmed that different extinction behaviors were produced through chemical and physical interactions that occurred under lean(rich)-lean(rich) condition.

Paper ID: 365

Investigation of influence of chemical kinetics mechanisms for hydrogen jet flame in a vitiated co-flow

Yuyang Zhang (Xi'an Jiaotong University), Hao Zhao (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University), Yingjia Zhang (Xi'an Jiaotong University)

The numerical simulation research was carried out on the hydrogen jet flame in a vitiated co-flow, using the large-eddy simulation method, the distributions of velocity, temperature and component concentration during jet development, ignition and combustion process had been study. Five detailed chemical kinetics mechanisms of hydrogen were used to investigate the influence of chemical kinetics mechanisms for numerical simulation result. The axial and radial data of simulation results of all five mechanisms were matched well with experimental data. The ignition characteristic and species distribution were strongly influenced by different detailed mechanisms. Through reaction pathway analysis and sensitivity analysis, the reason for the differences of simulation result is mainly depended on competitive differences for H atom of two reaction pathways ($H+O_2 <=> HO_2$, $H+O_2 <=> O+OH$) between five detailed mechanisms. Detailed mechanisms with linear-changing reactivity obtained by modifying key reaction parameters of KONNOV mechanism, were used to research the effect of mechanism to flame structure variation of hydrogen jet, and the jet flame transitioned from attached flame to lifting flame with the decrease of high temperature mechanism activity.

Paper ID: 366

On the unified modeling of the hydraulic resistance-driven and Shchelkin-type laminar flame acceleration in channels

Canruo chen (Tsinghua University), Damir Valiev (Tsinghua University)

Two distinctive modes of flame acceleration, hydraulic resistance-driven mode and Shchelkin-type mode, as well as an intermediate one, are analyzed numerically in planar 2D channels. Quasi-steady flame propagation regimes are obtained as well. The characteristic behaviors and dominant mechanisms for each mode are discussed in detail. Two criteria were proposed to classify the flame acceleration regimes. The flame acceleration regimes are mapped in the regime diagram for a range of channel widths and gas expansion coefficients.

Paper ID: 367

Numerical investigation on the flame behaviors in a mesoscale channel of one backward-facing step

Jyun-Hao Huang (National Sun Yat-sen University), Hsu Sheng-Yen (National Sun Yat-sen University)

Flame behaviors in mesoscale backward-facing channel are numerically investigated under isothermal

condition (300K) at walls. In the two-dimensional channel without symmetric assumption at centerline, four types of flame behaviors are found: 1.) steady convex flame, 2.) steady concave flame, 3.) simple oscillating flame, and 4.) complex oscillating flame. Above the flashback velocity, the convex flame exists steadily. With the increase in flow velocity, the flame becomes concave to the upstream and is stabilized by the wall-quenching effect of backward-facing steps. If further increasing the flow velocity, the flame becomes unstable and oscillates periodically due to the interaction of the flame instability and the stability of symmetric flow in backward-facing channel. The oscillating frequency decreases with the increase in flow velocity. Furthermore, the occurrence of complex oscillating flame at high flow velocities is attributed to the asymmetric flow pattern in backward-facing channel. In addition, some complex dynamic flame behaviors are also found in the backward-facing tube at higher flow velocities before extinguishing.

Paper ID: 369

Theoretical study on the tert-butyl hydroperoxide pyrolysis reaction

Yingjia Zhang (Xi'an Jiaotong University), Binxu Pu (Xi'an Jiaotong University), Qian Zhao (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University)

Tert-Butyl Hydroperoxide (TBHP, $(CH_3)_3COOH$), an alkyl organic peroxide compound, plays an important role in measuring the rate coefficients of ȮH + fuels because the O-O bond can easily break. In this process, TBHP pyrolysis reaction is the most sensitive reaction for ȮH radical generation, obtaining accurate kinetic parameters is the most important to construct TBHP mechanism model. However, different mechanisms have great differences in predicting the ȮH evolution of TBHP pyrolysis at $T > 1000$ K and the pressure-dependence is also not considered. In this study, the potential energy surface of TBHP pyrolysis was constructed at the CCSD(T)/cc-pVTZ//M06-2X/6-311G(d,p) and the CASPT2(2e,2o)/cc-pVTZ//CASPT2(2e,2o)/6-311G(d,p) level, four new reaction channels were found. Then the rate coefficients of TBHP pyrolysis reaction were obtained using the RRKM/ME method at $T = 298 – 2000$ K, $p = 0.0001 – 10$ MPa. The current calculated results are in good agreement with the experimental data. The temperature-dependence of the target reaction was reevaluated, and it shows seemingly ignorable pressure-dependence at low temperature ($T < 700$ K). However, the pressure-dependent behavior of this reaction system still needs to be considered at high temperature ($T > 900$K) and low pressure ($p < 1$ MPa).

Paper ID: 372

Numerical analysis of the effect of soot radiation on the wall temperature of the combustion chamber

Zhengzhe Fang (Beihang University), Zhang Chi (Beihang University), Bosen Wang (Beihang University), Chunhua Yang (Beihang University)

The strong heat transmission in the aero-engine combustion chamber leads to a significant challenge to the wall cooling design for the flame tube. The near-blackbody radiation from the soot has the potential to significantly increase the heat load on the wall. The heat load of soot radiation and its relative effect comparing to that of heat convection are obtained by analysis of the numerical simulation results. The Moss-Brookes soot model and the discrete coordinate radiation model (DOM) coupled with the steady flamelet model are used to capture the heat transmission in a non-premixed spray combustion chamber. The grid convergence of the numerical model is demonstrated and the accuracy of the model is validated based on the experimental

measurements of the wall temperature of the flame tube. The heat transfer loads of convection and radiation are quantified based on the converged and verified numerical simulations. The analysis demonstrates that soot radiation can improve the accuracy of the prediction of the flame tube temperature by up to 7%. The radiation heat load accounts for 24% of the total heat transfer to the tube wall for the equivalence ratio of 0.25 which decreases to 17.6% as the equivalence ratio is reduced to 0.12. Soot radiation for the higher equivalence ratio accounts for 30% of the total radiation. This quantitative analysis can give a direct view of the influences of soot and radiation on the flame tube wall and provide a reference for the cooling design.

Paper ID: 373

Application of quantitive Raman spectroscopy to turbulent flames of H_2/N_2

Andrew R Macfarlane (Sydney University), Assaad Masri (Sydney University), Matthew J Dunn (The University of Sydney), Hao Tang (KAUST), Gaetano Magnotti (KAUST)

This paper presents line-Raman/Rayleigh measurements of temperature and stable species collected in turbulent flames of H_2/N_2 = 40/60 issuing into the Sydney inhomogeneous piloted burner. Two flames are studied having the same bulk jet velocity of U = 69 ms^{-1} and equivalence ratio of φ = 4.76, yet different compositional inhomogeneity. One flame has homogeneous inlets, a recess distance of L_r= 300 mm, and the other has incomplete mixing at the jet exit due to shorter recess, L_r=25 mm. Measurements of temperature and the mass fractions of O_2, N_2, H_2O and H_2 reveal significant differences in the mixing, reaction and mixture fraction profiles between the two flames. For the compositionally inhomogeneous case (L_r =25 mm), there is significant unreacted gas mixing due to turbulence, at the outlet. This flame develops to a diffusion flame profile at tendiameters downstream of the exit. Conversely, for the homogeneous case with L_r = 300, the flame burns in a diffusion manner at the outlet with a small change in temperature and the mixture fraction relationship downstream. A comparison between a flamelet model using mulitcomponent diffusion and unity Lewis number reveal that the turbulent flames do not necessarily follow the laminar flamelet profiles.

Paper ID: 374

Thermal performance of fire blankets for protection against WUI fires

Robin Neupane (Case Western Reserve University), Ankit Sharma (Case Western Reserve University), Jonathan Fu (Case Western Reserve University), Ya-Ting T. Liao (Case Western Reserve University), Fumiaki Takahashi (Case Western Reserve University)

The recent rise in wildfire hazards due to climate change has been a serious concern for many countries across the globe. Experimental studies on protection against wildfires provide a better understanding of the wildfire characteristics and help to formulate fire hazard mitigation strategies. In this study, a series of bench-scale experiments have been conducted to determine the effectiveness of fire blankets in Wildland Urban Interface (WUI) fires. First, ASTM D4108 standard determines the thermal protective performance (TPP) rating of fire blankets from different fabric groups. Secondly, to evaluate the thermal performance of fire blankets against WUI fires, a direct flame contact using a Meker burner and a pine wood block are used as a common construction material of houses located in WUI. The TPP test rig is modified to determine the temperature distribution at different wood depths and heat flux penetrated through the wood block. The charring rates of wood blocks protected by different fire blanket configurations are compared. Double layered fire blanket

configuration results in a slow charring rate even after a long exposure to a given heat flux, demonstrating that fire blanket can be an effective strategy for fire protection of houses/buildings and equipment located in WUI.

Paper ID: 375

Investigation on the opening location affecting the delay time of backdraft

Chia Lung Wu (Chang Jung Christian University), Carvel Ricky (University of Edinburgh), Wen-Yen Juan (National Cheng Kung University)

Backdraft is a special phenomenon in fire research; the delay time of occurrence has been of interest in recent years as this influences the efficiency of firefighting. This paper investigates the location of the opening and whether it affects the delay time of backdraft. Results show that the location of the opening dramatically controls the delay time. The central opening demonstrates about 55-60 % delay time compared to the upper and lower location. Also, the warmer the room, the more violent backdraft will be. This provides insight into the firefighting and cooling strategy when ventilation-restricted compartment fire occurs.

Paper ID: 376

Further insights into the cascade utilization of chemical energy

Wu Honghuan (Xi'an Jiaotong University), Qian Zhao (Xi'an Jiaotong University), Wenlin Huang (Xi'an Jiaotong University), Wuchuan Sun (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University), Yingjia Zhang (Xi'an Jiaotong University)

The research of the new generation energy power system focuses on extending the concept of energy cascade utilization to chemical energy and the conversion process of chemical energy to physical energy for achieving higher thermal efficiency. In this study, the basic principles of the cascade utilization of chemical energy are further explored. The relationship between exergy destruction and the free energy change during the energy conversion process is established to clarify the essence of exergy destruction from chemical reactions. On this basis, we propose an overall regulation principle to reduce the exergy destruction during chemical reactions and reveal the intrinsic mechanism of the cascade utilization of chemical energy. It is suggested that the combination of a series of endothermic reactions can be designed for different cases to maximize the work potential of the chemical energy of fuel.

Paper ID: 377

Laser absorption diagnostics of OH concentration time-histories during dimethyl ether (DME) oxidation

Xin Zhang (Xi'an Jiaotong University), Zilong Feng (Xi'an Jiaotong University), Yufan Zhang (Xi'an Jiaotong University), Zuohua Huang (Xi'an Jiaotong University), Yingjia Zhang (Xi'an Jiaotong University)

The concentration time-histories of OH during DME oxidation were measured behind reflected shock waves using narrow-linewidth ring-dye laser absorption of R1(5) line at 306.7 nm (for 1.5 atm) and near the R-branch head at 306.47 nm (for 15.5 atm) of the OH A–X (0, 0) system. The mixtures of DME (1500 ppm)/O2 in Ar with equivalence ratios of 0.5, 1.0 and 2.0 were shock-heated to temperatures of 1188–1827 K and pressures of about 1.5 and 15.5 atm. The obtained OH time-history data were thoroughly compared with the predictions of four representative kinetic mechanisms to assess their performance. Sensitivity analyses of DME were

performed to clarify the OH evolution behavior and screen out the dominant reactions. Rate constants of selected reactions were recommended for further investigation to improve the model ability. The new measurement of OH concentration time history provides a microscopic validation target for the DME kinetic model at high temperatures. To our knowledge, current results are the first quantitative measurements of OH time-histories during high-pressure oxidation of DME, and it is clearly valuable in developing more accurate kinetic models of DME under engine-relevant conditions.

Paper ID: 378

Ozone-assisted low-temperature oxidation of *iso*-butane in a jet-stirred reactor

Long Zhu (University of Science and Technology of China), Qiang Xu (University of Science and Technology of China), Bingzhi Liu (University of Science and Technology of China), Zhandong Wang (University of Science and Technology of China)

Ozone is a strong oxidizer that can be used to accelerate and control the combustion process. By ozone addition, it is possible to explore the combustion kinetics of unreactive fuels under milder conditions, such as lower temperature and pressure. In this work, ozone-assisted low-temperature oxidation of *iso*-butane was performed in a jet-stirred reactor (JSR) at atmospheric pressure in the temperature range of 350 to 800 K. The reaction started as low as 450 K, which corresponded with the window of ozone decomposition, and the negative temperature coefficient (NTC) behavior was also observed from 650 to 750 K. More than twenty species were measured by synchrotron vacuum ultraviolet photoionization mass spectrometry (SVUV-PIMS) and gas chromatography (GC), and some intermediates have not been reported before during the oxidation of iso-butane, such as ketohydroperoxides. AramcoMech2.0 and a modified NUIGMech1.1 were tested against the present measurements, both of which overpredicted the low-temperature reactivity of *iso*-butane after 650 K.

Paper ID: 380

Lift-off and stabilization characteristics of turbulent autoigniting partially premixed NH_3+H_2 flames

Matthew J Dunn (The University of Sydney), Andrew MacFarlane (The University of Sydney), Assaad Masri (The University of Sydney)

This paper explores the impact of increasing NH_3 content in NH_3+H_2 partially premixed flames issuing into a hot coflow. NH_3 and H_2 have different chemical reactivities, exhibited by large differences in autoignition delays and laminar flame speeds. Temporal and spatial flame structure and lift-off height dynamics are explored using high-speed chemiluminescence imaging. Statistics on the lift-off height are reported for three hot coflow temperatures and NH_3 percentages in the fuel stream from 0% up to a maximum of 60%. NH_3 addition above 20% for the conditions explored is found to have a strong impact on the lift-off height, to a similar degree that the hot coflow temperature has.

Paper ID: 381

Ammonia/hydrogen mild combustion in a cyclonic burner

Giancarlo Sorrentino (CNR-STEMS), Giovanni Battista Ariemma (STEMS-CNR), Pino Sabia (CNR-STEMS), Raffaele Ragucci (STEMS-CNR), Mara de Joannon (STEMS-CNR)

In the present scenario related to the energy transition, fuel-flexible technologies for clean power generation

and propulsion is of paramount importance. In this context, ammonia is considered as a key decarbonized energy carrier, due to its very high hydrogen-density and well-established production processes. MILD Combustion already proved to be a very effective technology in converting ammonia in terms of stability and emissions performance. Despite that, the utilization of fuel enhancers in MILD Combustion conditions can be useful to further improve the process characteristics. The present work focuses on the combustion performance of ammonia/hydrogen blends. Experimental investigations were performed at 7 kW in a cyclonic-flow chamber operating under MILD Combustion conditions. NH_3/H_2/air mixtures oxidation was characterized in terms of process stability, operational temperatures and NOx emissions, as a function of the equivalence ratio and %H2 in the fuel mixture, in order to identify the best operative conditions for NH_3/H_2 stable combustion. Results confirmed the MILD Combustion effectiveness for NH_3/H_2 blends conversion, with reasonable NOx emissions. H2 widens the stable operational region for NH_3 oxidation, because of the boosted OH production, that also increases the NH_3 yield to NO, thus entailing higher NOx emission than the pure NH_3.

Paper ID: 382

Co-combustion characteristics of solid waste and coal

Shuhn-Shyurng Hou (Kun Shan University), Chung-Yao Hsuan (Kun Shan University)

The purpose of this study is to investigate the co-firing characteristics of sewage sludge (generated during wastewater treatment) and coal. Waste sludge contains many combustible components and is considered as a potential biomass fuel as a renewable energy source. Combustion characteristics of sewage sludge, Australian sub-bituminous coal, and their blends with different blending ratios (sludge/coal = 80/20, 50/50, 20/80 by weight) are explored under air combustion conditions via thermogravimetric analysis. In addition, the combustion heating performance and emissions of pure coal and 20% sludge + 80% coal are carried out with a 300 kW_{th} industrial furnace. The results of furnace combustion experiments show that under the condition of minimum excess oxygen combustion, and at a fixed heat release rate, there is no flame instability, and the temperature of the radiant zone of 20% sludge blended fuel is slightly higher than that of pure coal combustion, but the difference is not significant. It is verified that burning the pulverized sludge/coal blend with 20% substitution ratio exhibits similar furnace performance and low CO emissions. However, co-firing 20% pulverized organic sludge and 80% pulverized coal has slightly higher NO and SO_2 emissions.

Paper ID: P0101

Theoretical investigation for reaction mechanism of Al/CO/O_2 system

Nozomu Yonetani (Toyohashi University of Technology), Tatsuo Oguchi (Toyohashi University of Technology)

The reaction mechanism for the oxidation of Al in CO atmosphere is investigated theoretically by using quantum chemical calculations. The potential energy for stable molecules such as reactants, reaction intermediates, and products on the reaction potential surface were calculated using CBS-QB3 method. Some transition states or potential surfaces for recombination reactions were also investigated. The elementary reaction of Al with CO was examined and AlCO was found as the only major product. The self-reaction of AlCO was also examined and $(AlCO)_2$ product was found. The reaction of Al with AlCO formed two type of Al_2CO products. Al_2CO can also be formed from the reaction of Al_2 with CO. However, the reaction path for

the formation of pure oxidation products such as AlO could not be found in this system. AlO + O_2/CO reactions were also investigated for the construction of oxidation reaction modeling for Al/CO/O_2 system. In the high-temperature range, it was found that AlO_2 is an important intermediate in an oxygen-rich environment.

Paper ID: P0201

Preparation of nano-thermite by aluminum nanoparticles containing triphenylphosphine protective layer

You-Chi Jian (National Kaohsiung University of Science and Technology), Wan-Lien Hsu (National Cheng Kung University), Chao-Wei Huang (National Cheng Kung University), Ming-Hsun Wu (National Cheng Kung University), Chia-Ting Lin (National Chung-Shan Institute of Science and Technology)

In this study, triphenylphosphine was used as a protective layer to prepare shelled nano-aluminum particles, and the above-mentioned self-made aluminum powder was directly mixed to synthesize nano-thermite. An X-ray diffractometer (XRD) and analytical field scanning electron microscopy (AFE-SEM) were used to determine its composition, shape, and particle size. The ignition properties of thermite were also examined in open space. The results indicate that nanosized aluminum particles were synthesized successfully and exhibited the exothermicity of partial nano-aluminum particles.

Paper ID: P0301

Development of a TDLAS system for quantifying CO_2 concentration in combustion gas

Chun-Wei Wu (National Cheng Kung University), Bao-Wen Chang (National Cheng Kung University), Ming-Hsun Wu (National Cheng Kung University)

Tunable diode laser absorption spectroscopy (TDLAS) is a non-intrusive and instantaneous method for measuring species concentration as well as temperature in combustion exhaust gas. It has been successfully employed for measurements of methane, carbon dioxide, carbon monoxide, water vapor, ammonia, etc. under various circumstances. Studies have also shown that pressure and velocity can be resolved with this approach. In this study, a TDLAS system based on a distributed-feedback(DFB) laser with a centerline wavelength of 2004 nm was set up for quantifying CO_2 concentration in exhaust gas from a combustion system. Both direct absorption spectroscopy (DAS) and wavelength modulation spectroscopy (WMS) were applied for signal processing. Calibration of gas concentration was performed using CO_2/air mixtures prepared with high precision mass flow controllers. A custom-made cylindrical gas cell in which multiple reflections occur along the circumference of the gold-plated inner wall of the cylinder has been designed and constructed to enhance the sensitivity of the system. A total light path of 2.55 m can be achieved with the 7.5 cm diameter cell. In addition to being used for calibration, the cylindrical cell is intended to be directly mounted on the outlet of the combustion chamber for in-situ measurement after removing the front and the back covers. Experiments will be carried out in a bench scale combustor system to validate the TDLAS system, and the data will be verified using a NDIR gas analyzer. The system will be eventually integrated to a test rig for gas turbine combustors.

Paper ID: P0302

Mid-infrared interband cascade laser sensor for temperature and CO concentration measurement in laminar premixed flames using heterodyne phase-sensitive dispersion spectroscopy

Weitian Wang (Tsinghua University), Zihao Song (Tsinghua University), Zhenhai Wang (Tsinghua University), Ning Zhu; Xing Chao (Tsinghua University)

Dispersion spectroscopy-based laser diagnostic techniques bear the same advantages as absorption-based techniques, such as being in situ, non-intrusive, highly quantitative, and the intrinsic advantage of being immune to absolute power fluctuations. The baseline-free nature of phase detection makes dispersion-based laser sensors potentially powerful for combustion applications. We develop a 4854nm mid-infrared interband-cascade-laser (ICL) sensor based on heterodyne phase-sensitive dispersion spectroscopy (HPSDS) technique for CO sensing in flame. While the experimental setup is similar to tunable diode laser absorption spectroscopy (TDLAS), an additional high-frequency modulation signal at 900MHz is superposed upon the injection current of the laser diode. Such direct modulation of laser induces both intensity and frequency modulation, thus generates a three-tone beam. Absorption and dispersion of the transmitting media can then be reestablished from the heterodyne beat signal at modulation frequency on a high-bandwidth photodetector. For proof-of-concept demonstration, CO temperatures and concentrations in a laminar premixed methane/air flame under different equivalence ratios (ϕ) are measured at 100Hz and compared with TDLAS and simulation results, which shows a good agreement. The relative differences of averaged CO temperature and concentration between TDLAS and HPSDS results for ϕ=1.0~1.3 are <6% and <10%, respectively. The noise-equivalent dispersion of the sensor is estimated to be 0.0193rad in a single-shot measurement, corresponding to a noise-equivalent concentration of 59.46ppm·m. The results indicate that HPSDS technique presents a useful and practical diagnostic tool complementary to laser absorption techniques, with unique advantages in harsh combustion environments involving significant laser transmittance fluctuations.

Paper ID: P0303

Sorting and decontamination of e-waste plastics

Pallab Das (Nanyang Technological University), Jong-Min Lee (Nanyang Technological University)

E-waste plastics are often found to be contaminated with toxic metals (Hg, Cd, Cr, and Pb) and brominated flame retardants (BFRs), which can be traced back to the additives appended during manufacturing1. The sources of contamination can be traced to the additives added during manufacturing or from the surrounding environment. One of the challenging issues of recycling these plastics is segregating them with respect to their resin type or type of contamination. Recycling these plastics poses a significant challenge, especially when it comes to segregating them based on the type of contamination or resin. To address this challenge, we have developed a fast and efficient sorting facility that uses laser-induced breakdown spectroscopy (LIBS) and machine learning algorithms to identify and classify various plastic types with up to 95% accuracy. To decontaminate the contaminated plastics, we have developed solvent-based extraction processes such as microwave-assisted extraction (MAE), ultrasonic-assisted extraction (UAE), and dissolution and reprecipitation (DR) processes. We have used weak acid solvents to remove Pb from the PVC obtained from the electrical cables[2], while safe organic solvents were screened to identify suitable solvent combinations for extracting BFR from styrene-based plastic matrices found in different types of waste electrical and electronic

equipment (WEEE) bodies.

Paper ID: P0401

Study of DC electric field on flame behavior and emission with hydrogen and methane fuel in co flow non premixed flame

Byeong Hun Seok (Korea Institute of Industry Technology), Jun Seok Kim (Korea Maritime & Ocean University), Sung Hwan Yoon (Korea Maritime & Ocean University), Jungho Whang (Yonsei University), Dae Geun Park (Korea Institute of Industry Technology)

The effects of DC electric fields on flame behavior and emission were experimentally investigated for non

Premixed hydrogen/ m e thane flames in a co flow burner. The fuel based on methane added hydrogen mole fraction 10%, 30%, 50%, and the fuel flow s velocit ies were 3cm/s, 6.3cm/s, and 8cm/s. To apply DC electric fields, the high voltage terminal and the ground terminal were conn e c ted to the fuel nozzle and upper mesh which is above the flame. Here, the DC voltages were from E_{dc} = 10 kV to 10 kV. The flame height and yellow luminosity from soot particles were decreased adding the hydrogen. We observed that the flame subjected to the DC electric fields moved toward lower potential side with showing stable and oscillating flame due to the Lo rentz force acting on the positive ions in flames. To clarify relation between flame and DC electric fie ld, the mie scattering method was adopted for flow visualization with TiO_2 particles. The concentration of CO, CO_2 , and NO_X with adding hydrogen and the electric fields, the gas analyzer set (Testo 350K) was installed at an exhaust pipe. As the results, th e emissions are insignificantly changed with adding hydrogen mole fraction. And the emission s of CO_2 , NO_X are reduced with both positive and negative electric fields. The emission of CO is monotonously increased from negative to positive voltages. The deta iled flame/flow behavior and emission characteristics with hydrogen and DC electric fields were discussed

Paper ID: P0402

Experimental and theoretical study of critical laminar burning velocity on the destabilization of ammonia planar flames propagating downwards in tubes transitioning to parametric instability

Jerric R. Delfin (Hokkaido University), Feng Guo (Hokkaido University), Osamu Fujita (Hokkaido University)

This work presents the experimental and theoretical study of self-excited parametric instability of $NH_3/O_2/N_2$ downward propagating flames in open-close tubes for the first time. Nonequidiffusive ammonia gas mixtures at different laminar burning velocities (S_L) at ϕ=0.8 and ϕ=1.2 were ignited and propagated in a combustion tube. Typically, at sufficiently high S_L, curved flames after ignition are planarized by acoustic standing waves that subsequently form cellular flames that oscillate twice the period of acoustic standing due to parametric instability. This work investigates the critical S_L for ammonia flames which is the minimum S_L where stable flat flames are not observed in transition to parametric instability during flame propagation. The effect of Lewis number (Le) on critical S_L is consistent with theory and experiments. The correction term (a function of Zeldovich number β and Le) applied to the analytical prediction of the range of acoustic velocities where stable flat flames are observed showed good agreement with experiments in determining the critical S_L. Comparative experimental and theoretical analyses on thermoacoustic instability between $NH_3/O_2/N_2$ and $CH_4/O_2/N_2$ downward propagating flames reveal that ammonia exhibits a narrower range of acoustic velocities

where stable planar flames occur and consequently lower theoretical and experimental critical S_L compared to methane even if ammonia flames have higher Markstein (*Ma*) numbers than methane flames at the same equivalence ratio and laminar burning velocity. Further study is expected on the investigation of ammonia and the quantification of the combined effect of several thermophysical properties of fuels on the instability of planar flames.

Paper ID: P0501

Investigation of flame-vortex interaction and combustion noise in a backward-facing-step burner

Ji Hun Yeo (Korea Advanced Institute of Science and Technology), Nam Il Kim (Korea Advanced Institute of Science and Technology), Hui Man Yang (Korea Advanced Institute of Science and Technology)

To investigate the relationship between the flame-vortex interaction and the combustion noise, many studies have been conducted with backward-facing-step (BFS) burners. It is known that the combustion noise driven by the BFS structure can be self-sustained, and the coherent frequencies can be detected as peaks in the noise power spectrum. In many previous studies, the flame oscillation and the flow field could be visualized using PIV (Particle Intensity Velocimetry) or measuring chemiluminescence emitted from the flame. In this study, we adopted some novel visualization methods, and periodic flame behaviors could be understood more clearly. Notably, in our BFS burner, the step-width and nozzle-width could be continuously varied. In addition, the sensitivity of these length scales on the combustion noise could be assessed. Experiments were mainly focused on the transition regime between laminar and turbulent flames. Periodic traces of the flames within the combustion space were depicted as contours for specific frequencies of the combustion noise. This contour was compared with the corresponding streamlines and the periodic location of the flames. We could understand how frequently the flame propagates into the recirculation zone and which parts of the flames generate the periodic flame behaviors. Some coherent trends were found regardless of fuels (C_3H_8 and CH_4) or their compositions, and the visualization results were used to investigate the mechanism of flame-vortex interaction and consecutive noise.

Paper ID: P0701

Numerical study of a Hhgh-pressure hydrogen tank burst at different heights from the ground and its hazards on humans

Dinesh Myilsamy (Pukyong National University), Paulo Cardozo Soares Amaral (Pukyong National University), Chang Bo Oh (Pukyong National University)

A numerical study was carried out to investigate the overpressure hazards of a 35 MPa, 72.4 L hydrogen tank burst at different heights from the ground. An open-source OpenFOAM CFD code was used to perform the numerical investigation. The numerical simulations were based on a fully-compressible unsteady Reynolds-Averaged Navier-Stokes (URANS) turbulence approach with a k−ω SST turbulence model, Peng-Robinson real gas equation of state and a one-step reaction eddy dissipation concept (EDC) combustion model. The high-pressure hydrogen tank burst at different heights from the ground was investigated using the validated numerical approach. The hydrogen tank burst scenarios are 0.0 m, 0.2 m, 0.5 m, 0.8 m, 1.0 m and 0.2 m with a 65° vertical tilt from the ground. The numerical predictions showed that the maximum overpressure magnitude and the blast impulse were affected by the tank burst height from the ground and its position. The

tank 0.0 m on the ground resulted in the strongest overpressure hazard in the radial direction, and the 0.2 m with a 65° vertically tilted tank burst showed the strongest impulse hazards at farther distances in both the axial and radial directions. The overpressure hazards in the axial direction increase with the increasing tank height from the ground. The overall pressure-impulse diagram showed that the blast hazards in the radial direction are significantly stronger than in the axial direction of the hydrogen tank.

Paper ID: P0801

The combustion process of a single wood pellet under convective oxy-fuel atmospheres with steam addition

Hsien-Tsung Lin (National Cheng Kung University), Guan-Bang Chen (National Cheng Kung University), Yei-Chin Chao (National Cheng Kung University)

Oxy-biomass combustion combined with carbon capture and storage technology enables negative CO_2 emissions in power plants. However, the combustion of biomass pellets in wet flue gas recirculation scenarios remains unclear and there is scarce literature. In this study, the combustion process of a single wood pellet under 550°C isothermal convective air stream and $O_2/CO_2/H_2O$ atmospheres were explored. In addition, flame images, combustion characteristics times, particle temperature, and mass loss evolution were simultaneously measured. The results showed that stabilized volatile flame around the wood pellet appeared when $O_2 \geq 21\%$. With H_2O partially replacing 20% of CO_2 at oxy-21%, the ignition delay time of char (ti,char) and flame (ti,flame), char combustion duration (tchar), and total combustion time (ttotal) reduced 7.89%, 6.02%, 17.98%, and 16.05% was found, respectively. It is attributed that H_2O possesses higher thermal diffusivity (2.1 times) and O_2 mass diffusivity (1.61 times) than CO_2, which promotes combustion. In particular, volatile flame burning duration (tflame) significantly elevated 266% due to char-H_2O gasification reaction shifting carbon to flammable fuels to sustain the flame. The results of tchar under $O_2/CO_2/H_2O$ atmospheres with 15–33% O_2 and 0–50% H_2O combination demonstrating that reaction rates follow char-O_2 > char-H_2O > char-CO_2. Furthermore, ttotal of wood combustion under 27%O_2/73%CO_2 and 21%O_2/50%H_2O/29%CO_2 conditions was comparable with that in air. This study provides insights into biomass ignition and combustion fundamentals, which is conducive to its application in industrial oxy-combustion systems.

Paper ID: P0802

Experimental study of coal/ammonia co-firing using bench-scale furnace system

Taeyoung Chae (Korea Institute of Industrial Technology), Won Yang (Korea Institute of Industrial Technology), Jaewook Lee (Korea Institute of Industrial Technology), Kyoungil Park (Korea Electric Power Corporation)

The experiment was conducted based on 80kW heat input, and the ammonia co-firing rate was increased by 5, 10, 15, and 20%. As the co-firing rate increased, the NOx in the combustion gas tended to increase. However, in this study, NOx production could be suppressed by controlling the flow rate. Under certain conditions, NOx showed a trend to decrease. As a result of the experiment, it could be seen that NOx increased as the ammonia co-firing ratio increased, but the NOx generated differed depending on the ammonia input method. As a result of the study, NOx can be reduced in case of ammonia is directly injected into the reduction area.

Paper ID: P0901

Relationship between mixing ratio and flame spread rate of cellulose/polypropylene composites

Takuya Yamazaki (Toyohashi University of Technology), Taisuke Kawasaki (Toyohashi University of Technology), Koki Matsumoto (Fukuoka University), Daiki Matsugi (Toyohashi University of Technology), Tsuneyoshi Matsuoka (Toyohashi University of Technology), Yuji Nakamura (Toyohashi University of Technology)

The effect of the pyrolysis characteristics of the cellulose/polypropylene composites on the flame spread rate has been experimentally examined. In the pyrolysis reactions in biomass/plastic composite materials such as cellulose/polypropylene composites, the amount of pyrolysis gases is enhanced or suppressed due to the competitive pyrolysis reactions. However, the relationship between the production of the pyrolysis gases and the flame spread rate in a biomass/plastic composite has not been clarified. To reveal the influence of enhancement or suppression of pyrolysis gas production on flame spread rate, downward flame spread tests and pyrolysis gas chromatography mass spectrometer Py-GC/MS were conducted for a thin sheet of cellulose/polypropylene composites. The flame spread rate dramatically decreases with the increase of the cellulose/polypropylene ratio in the range of 10 – 30 wt.%, whereas slightly fluctuates in the range of 40 – 100 wt.%. To examine the decreasing trend of the flame spread rate, the adiabatic flame temperature was estimated with Chemkin-Pro assuming the primary pyrolysis gas compositions derived by the Py-GC/MS. The comparison between the flame spread rate and the flame temperature implies that the fluctuated trend of the flame spread rate in the range of 40 – 100 wt.% is attributed to the decrease of the flame temperature due to the competitive pyrolysis reactions. On the other hand, the abrupt decrease of the flame spread rate can be caused by other reasons, for example, dripping the polypropylene polymers. Further discussion will need to consider the dripping.

Paper ID: P0902

Experimental observations of downward flame spread along thin wire in various gravity fields using a centrifuge

Yusuke Konno (Hokkaido University), Shoryu Ishikawa (Hokkaido University), Nozomu Hashimoto (Hokkaido University), Osamu Fujita (Hokkaido University)

In the context of recent trends in the international community regarding human space exploration, the authors have been working on the FLARE3 project (successor project of Flammability Limits at Reduced Gravity called FLARE) since 2021 to improve the fire safety of manned space facilities to be built on the Moon and Mars. The project aims to develop a combustion test system that can reproduce the partial gravity, low pressure, and high oxygen concentration environments that will be explored in future manned space missions, and to establish a test facility on the ISS Japan Experimental Module “Kibo” that can verify flammability of various materials. The basic concept of the R&D in the project is to reproduce combustion phenomena in an arbitrary gravitational field by utilizing the centrifugal force acting on an object in uniform circular motion. This study discusses the effectiveness of observing flame spread phenomena along the solid materials in centrifuges as a basis for spacecraft fire safety. Thin wires which consist of a metallic core and polymer insulation are used as test samples. A sample is supported vertically in a chamber at 120 mm apart from the rotation axis. The upper end of the sample is ignited by a hot wire and subsequent downward flame spread under varied centrifugal

force is observed. Based on experimental observations, the effects of centrifugal and Coriolis forces on flame spread rate and flame shape are discussed, and the validity of using centrifuges to investigate gravity effects on material flammability is discussed.

Paper ID: P1001

Fluidized properties of a mixture of basic oxygen furnace slag with iron ore in a fluidized-bed chemical looping system

Cetera Chen (Industrial Technology Research Institute), Seng-Rung Wu (Industrial Technology Research Institute), Heng-Wen Hsu (Industrial Technology Research Institute)

The goal of this research is to develop fluidized-bed chemical looping system using BOF slag based material as an oxygen carrier and methane as fuel for heat production. Because BOF slag contains 21wt.% Fe2O3, which is insufficient to effectively convert methane, mixing BOF with iron ore is a direct way to increase oxygen release of oxygen carrier. In this study, fluidized phenomena of BOF slag and iron ore were observed on a fluidized bed test facility. The results showed, minimum fluidized velocity of iron ore with diameters of 177~297μm was about twice that of BOF slag. Mixture of BOF slag and iron ore with diameters of 177~297μm gave poor fluidized mixing, and resulted in a separating layer distribution of BOF slag and iron ore. Iron ore with diameters of 150~210μm gave the same minimum fluidized velocity as that of BOF slag with diameters of 177~297μm. Consequently, BOF slag with diameter of 177~297μm mixing with iron ore with diameter of 150~210μm indicated well fluidized mixing. This study presented a proper oxygen carrier composition of BOF slag and iron ore, to promote methane conversion rate of chemical looping system.

Paper ID: P1002

Parametric study of radiant tube burner by CFD modeling

Chien-Shun Lin (National Cheng Kung University), Chien-Chou Tseng (National Cheng Kung University), Ming-Hsun Wu (National Cheng Kung University)

In order to investigate the damage inside radiation tube burner (RTB) caused by uneven temperature distribution and reduce the emission of flue gas after combustion, the radiant tube insert (RTI) has been installed at the end of the RTB and simulated by CFD model. The purpose is to increase the disturbance of the exhaust gas at the end of the RTB, which increases the heat transfer effect near the tube wall and the temperature. In addition, a catalyst coating was added to the surface of RTI to reduce the emission of pollutants at the exit of RTB, and the removal effect of carbon monoxide through the catalyst insert was analyzed. In order to reduce the computational cost, we divided the simulation into two parts: the overall RTB combustion simulation and RTI. In order to facilitate the parametric analysis and the subsequent testing of different porosity of RTI, a porous media model was used instead of a solid honeycomb RTI. The results showed that the implement of RTI could increase the temperature of the RTB wall in the back section by about 30 degrees, and the removal rate of carbon monoxide by the oxidation catalyst could reach about 70% on average, depending on the configuration of RTI.

Paper ID: P1003

Effects of unburned gas humidification on flashback, NOx emission, and thermal efficiency in boilers with hydrogen premixed flame burners

Hui Man Yang (Korea Advanced Institute of Science and Technology), Nam Il Kim (Korea Advanced Institute of Science and Technology), Ji Hun Yeo (Korea Advanced Institute of Science and Technology)

Hydrogen is attracting interest as a carbon-free fuel to replace traditional hydrocarbon fuels. However, in the case of boiler systems, premixed hydrogen flames induce severe flashback or enhanced NOx emission. Operating burners at sufficiently fuel-lean conditions could suppress flashback and NOx emissions. However, the thermal efficiencies of the boiler systems might decrease significantly. To solve these problems simultaneously, water vapor recirculation technology was suggested. In this study, water vapor was supplied to the unburned mixture, and its effects on flame stabilization and NOx emission were investigated experimentally while overall thermal efficiency was estimated theoretically. It was found that the flashback through the perforated plate could be reduced by unburned gas humidification mainly due to the reduction of the burning velocity. The NOx emission could also be reduced due to the thermal dilution effect of water vapor. On the other hand, the thermal efficiency of a boiler system decreased up to 5% point at the stoichiometric condition when the methane was replaced by hydrogen. Nevertheless, the unburned gas humidification increased thermal efficiency drastically by enhancing moisture condensing and reducing the maximum flame temperature. Conclusively, it was shown that an unburned gas humidification cycle could be a promising technique.

Paper ID: P1004

Numerical simulation of ammonia combustion in a 760kW combustion furnace

Kenji Tanno (Central Research Institute of Electric Power Industry), Hiroaki Watanabe; Takayuki Nishiie; Kazuki Tainaka (Central Research Institute of Electric Power Industry), Hiroyuki Nishida (Central Research Institute of Electric Power Industry), Maromu Otaka (Central Research Institute of Electric Power Industry), Masayoshi Kimoto (Central Research Institute of Electric Power Industry)

Thermal power generation using ammonia as fuel is attracting attention as a CO_2-free power generation technology. In Japan, as the first step, a demonstration project is underway to co-fire coal and ammonia at a coal-fired power plant. In co-firing ammonia and coal, ammonia is co-fired in a burner or in a boiler. In this study, Large Eddy Simulation (LES) was performed for an ammonia combustion field with a burner developed for coal-combustion, assuming that coal and ammonia are co-fired in a boiler. For the turbulent combustion model, the flamelet generated manifold model (FGM) model was used. The NO concentration was separately calculated by solving the transport equation without using the flamelet database. Ammonia was injected through a nozzle in the center of the burner. Two-stage combustion was adopted for the combustion field, and the two-stage combustion rate is set at 30%. Numerical results showed the ammonia combustion characteristics in the combustion furnace. In the primary combustion zone, ammonia not only burns directly but decomposes into hydrogen. The hydrogen produced here is consumed in the two-stage combustion area by reacting with additional air. NO is actively produced in the higher temperature zone where hydrogen and air are reacting. However, NO decomposes in the strong reducing zone in the downstream. The numerical results for the relationship between NO concentration at the furnace outlet and air supply is in qualitative

agreement with the experimental results.

Paper ID: P1006

CO_2 emissions of combustion in plastic-IPGCC and plastic-IGCC

Beom-Hui Lee (Korea University), Seong-Kyun Im (Korea University)

The CO_2 emissions from the combustion processes in an integrated plasma gasification combined cycle (IPGCC) and an integrated gasification combined cycle (IGCC) were evaluated for plastic waste-to-energy recovery. Existing plastic treatment methods mainly include incineration, landfill, and recycling. These methods are closed-loop methods that the most of plastics are finally disposed in land or ocean. To prevent the environmental problems, chemical recycling such as pyrolysis and gasification of plastics have been suggested as the solution. In this study, NiO/Al_2O_3 was utilized as catalyst for comparing the CO_2 emission between IGCC and IPGCC. CO_2 converts to CO at the non-thermal plasma catalytic reactor, then H_2 and CO are combusted in the combustor. We modeled a DBD plasma reactor using kinetic modeling method. Moreover, Engineering equation solver was used to model the plastic gasifier, plasma catalysis unit, and combustion chamber. The effects of the quantity and temperature of the air and plasma catalyst unit on CO_2 production were investigated. The CO_2 emissions from IGCC was slightly higher than IPGCC in the range of the studied equivalence ratio (ER). As the temperature of air was increased, the reduction amount of CO_2 was decreased. The maximum reduction of CO_2 was observed when the injection temperature and ER were 900 K and 0.5, respectively. The results showed that the plasma catalyst reactor has advantages for reducing CO_2 emissions from the combustion process.

Paper ID: P1007

Study on the reforming of carbon dioxide/methane mixture with waste heat recovery

Wei-Cheng Chiu (Kun Shan University), You-Ming Chang (Kun Shan University), Cheng-You Wu (Kun Shan University), Cheng-Hsun Liao (Naval Shipbuilding and Development Center), Chun-Yi Kuo (Naval Shipbuilding and Development Center), Shuhn-Shyurng Hou (Kun Shan University)

In this study, using unconventional natural gas as raw material, the conversion of CO_2 and the production of syngas were studied via a self-developed waste heat recovery reformer. The unconventional natural gas was composed of methane and carbon dioxide. A series of tests were performed in a reformer with heat recovery for the reforming of unconventional natural gas. Controlled parameters included reactant feeding rate, CO_2/CH_4, O_2/CH_4 ratios and the operating temperature. The experimental results showed that increasing furnaces temperature could supply more energy for reforming and the concentration of H_2-rich syngas was enhanced. In the oxidation reaction process by air addition, part of the chemical energy released from the reaction provided the energy required for reforming reaction. Therefore, CO_2 conversion efficiency was increased by autothermal reforming at high CH_4 feeding rate and CO_2/CH_4 ratio. The oxidation heat released and gas hourly space velocity (GHSV) increased with the increase of O_2/CH_4 ratio. High O_2/CH_4 indicated that a large amount of energy was generated from the oxidation reactions. Moreover, the residence time decreased as the O_2/CH_4 ratio increased, and then the reforming efficiency was reduced.

Paper ID: P1008

Numerical simulation of CH_4/H_2 combustion in an industrial pilot scale heating furnace

Zong-Yu Pan (National Cheng Kung University), Fang-Hsien Wu (National Cheng Kung University), Guan-Bang Chen (National Cheng Kung University), Ming-Hsun Wu (National Cheng Kung University), Ta-Hui Lin (National Cheng Kung University)

Reacting flow simulations of an 100 kW scale heating furnace was carried out in the present study to explore the characteristics of non-premixed CH_4/H_2 combustion using an industrial swirl burner. Hydrogen enrichment has drawn extensive interests recently due to its potential on reducing CO_2 emission from a combustion device. But fundamental studies have shown that combustion temperature and NOx emissions increase when part of the hydrocarbon fuel like methane is replaced with hydrogen. Soot formation and combustion instabilities may also be altered with hydrogen addition. To reveal the effects of the hydrogen addition to the performance of industrial swirl burner, simulations are carried out using commercial CFD package (ANSYS Fluent). Grid size of the model for the 100 kW furnace was around 3 millions nodes, and Eddy Dissipation method with 3 steps reaction kinetics are employed for combustion modeling. Thermal NO and prompt NO models are enable in the simulation. Volumetric concentration of hydrogen in the fuel will be varied from 0 (methane) to 100 (hydrogen) will be investigated. Emphasis will be made on the influence of hydrogen content on flame length, thermal profile in the furnace and NO emissions.

Paper ID: P1009

Data-driven model for NOx emission control of a rod-mill furnace

Weidong Hsieh (China Steel Corporation), Tingshuo Chen (China Steel Corporation), Weiyu Chen (China Steel Corporation), Yihsien(China Steel Corporation)

A 40-year-old rod-mill furnace is facing a tremendous challenge due to stricter NOx emission regulations. The old NOx regulation was 120ppm at 6% O2 correction, while the new NOx regulation has dropped to 80ppm. The furnace must be able to run at 80ppm in order to renew its operating license. Though the operators can adjust the zonal air-fuel ratio to meet the requirement, they cannot adjust it constantly according to different operating conditions. Therefore, we have developed a data-driven model based on archived operating data such as furnace zonal air flow, fuel flow, furnace pressure, and flue gas measurements. The PyCaret package was used to facilitate the model building process and the XGBoost algorithm was selected to model the NOx. The model was validated off-line and an optimization method was proposed to advise the appropriate zonal air-fuel ratio combinations to reach the target NOx emission. By feeding in the real-time furnace operating data, the reheating furnace can then be controlled by the model and maintain low NOx operation. Online testing has shown that during model control, the NOx emission significantly dropped. Additionally, the flue gas O2 also dropped along with the increase of preheat combustion temperature, indicating better furnace efficiency and energy saving potential.

Paper ID: P1201

Design of a high-pressure spray combustion test rig for gas turbine combustors

Qi-Wei Zeng (National Cheng Kung University), Chen-Yu Lien (National Cheng Kung University), Ming-Hsun Wu (National Cheng Kung University)

Design of a high-pressure spray combustion test rig is presented in this work. Since the combustor of a gas turbine is a complex combustion device in which high-pressure and high temperature air from a compressor is mixed with lliquid sprayspray, visualizations of the atomization, mixing, and combustion processes in the chamber will be instrumental for the development and improvement of the combustor and injector designs An optically accessible test rig is also essential for the validation and refinement of simulations during the design process nowadays. The present design features a transparent test section with a double-layers configuration. The inner combustion chamber was made of a fused silica tube, and windows on the four sides of outer casing to allow optical diagnostics of flame dynamics. Maximum air temperature of 700 K, and flow rate of 0.1 kg/s can be achieved in the system. The maximum operating pressure of the test section i s 2 MPa. The pressure in the outer casing will be slightly larger than the inner combustion tube. Flow rate, pressure, and temperature can independently control on the rig. The flow rate can be adjusted through a high-pressure mass flow controller upstream of the electric air heater, in which the applied power determines the combustion air temperature. Pressure in the combustion test chamber can be adjusted using a cooled backpressure valve at the end of the test section. Fluid dynamic simulations will be performed to assist the design. For future gas turbine combustor tests, adapter design at the inlet of the test section that will enable easy interchange of burners will also be pursued.

Paper ID: P1202

Combustion instability characteristics with pilot burner operating condition in fractal grid low-swirl multi-nozzle combustor

Jinseong Kim (Center for Aerospace Engineering Research), Jihwan Ahn (Center for Aerospace Engineering Research), Keeman Lee (Center for Aerospace Engineering Research)

This study sought to understand the lean blowout(LBO) behavior of flames and the stability of flames according to the operating conditions of the pilot combustor in a low-swirl can-type combustor consisting of a pilot combustor and five nozzles. The grid generated turbulence of the the low-swirl injector used in the study has a fractal shape, and the dynamic state transition of the combustor was investigated by measuring the pressure perturbation inside the combustion chamber using a dynamic pressure sensor. As a result of investigating the change in pressure perturbation according to the operating load while changing the local equivalent ratio of the pilot combustor, the combustion instability that appears before the lean flammable limit is resolved as the operating load of the pilot combustor increases. As a result, it was found that the operation of the pilot combustor had an effect on the behavior of the flame cluster in the combustion chamber.

Paper ID: P1203

Development of a finite volume helmholtz equation solver for a large-scale combustion instability problems

Namsu Kim (Korea Institute of Energy Research), Young Tae Guahk (Korea Institute of Energy Research), Changbog Ko (Korea Institute of Energy Research), Taesong Lee (Korea Institute of Energy Research)

In this work, we present a new finite volume method-based Helmholtz equation solver designed to solve the thermoacoustic instability problem in practical combustion engines. The thermoacoustic mode in a combustor can be described by the pressure wave equation and a forcing term which accounts for the interaction between

thermodynamic, acoustic, and fluid processes. Compared to brute force computation of reacting flow in a complex combustor geometry, solving the inhomogeneous Helmholtz equation is a more cost-efficient method for predicting combustion instability. The solver discretizes the inhomogeneous Helmholtz equation using OpenFOAM, and the equation matrices are converted to the PETSc format to effectively utilize the large-scale nonlinear eigenvalue problem with state-of-art eigenvalue algorithms in SLEPc. To validate the implementation of the Helmholtz equation and flame response function models, a comparison of the analytic predictions to numerically computed wave frequencies was conducted. Finally, we simulate a thermoacoustic problem in a full-scale real combustor and compare the predicted acoustic frequencies and growth of the thermoacoustic mode with experimentally measured data. We also discuss the scalability and limitations of the solver.

Paper ID: P1204

Linear burn rate of SHP163 gel propellant

Yu-Jia Chen (National Cheng Kung University), I-You Tsai (National Cheng Kung University), Ming-Hsun Wu (National Cheng Kung University)

In this study , strand burner tests of SHP163 gel w ere carried out in a pressure chamber to investigate the burn rate of the liquid monopropellant after gelation using fumed silica SHP163 is a promising methanol/ hydroxylammoniu m nitrate (HAN based propellant , which ha s recently received great attention . With the addition of methanol to HAN aqueous solution, the burn rate is reduced and the abrupt burn rate surge in the transition zone between 1.1 and 2.1 MPa is mitigated . It has been found that similar effect can be achieved by the gelation of HAN aqueou s solution using hydrophilic fumed silica (CAB O SI L m5). To explore the effect of gelling SHP163 with CAB O SIL on the burn characteristics , strand burner experiments were conducted in a chamber filled with argon at pressure s between 0.1 and 3.1 MPa Influence of gellant concentration on the linear burn rate was also studied. Results showed that self sustained reaction propagation can be achieved in the gelled propellant all the way down to atmospheric pressure , while the reaction was not self sustainable for liquid SHP163 below 1. 1 MPa . T he linear burning rate of SHP163 gel is slightly higher than that of SHP163 liquid solution . T he pressure dependence index is 1.09 for the gelled SHP163 with 5% wt. CAB O SIL between 0.1 and 3.1 MPa. It has also been found that the burn rate decreases with gellant concentratio n at 3.1 MPa. Under 0. 6 MPa, the burn rate first increase then decrease with increasing amount of CAB O SIL in the propellant.

Paper ID: P1301

Electrolytic decomposition of HAN-based propellants under elevated pressures

Yu-Ting Chou (National Cheng Kung University), Guo-Zheng Yang (National Cheng Kung University), Ming-Hsun Wu (National Cheng Kung University)

The aim of this study is to explore the electrolytic reaction mechanism of 80 wt .% HAN under different electrolysis duration , pressures and voltages. Hydroxylammonium nitrate (HAN) is a low toxicity green liquid mono propellant that is expected to replace hydr azine in the space propulsion. However, HAN based propellant has relatively high ignition temperature and requires high temperature catalyst due to the higher reaction temperature. E lectroly tic decomposition may address the problems since self sustained de

composition can be initiated from any temperature w hile potentially consume s less power than thermal catalytic decomposition . E lectrolysis duration ranging from 0.25 to 5.0 seconds have been tested in the study using 80 wt ..% HAN under 0.6 MPa . Pressure and voltage investigated are from 0.1 to 4.1 MPa, and 40 to 60 V , respectively . High speed cameras a were used to record the reaction process, while the residual liquid was analy zed using FTIR ATR to clarify the mechanism of the electroly tic react ion. Based on the experimental results , the Violent bubbling was first observed on the anode side in the HAN solution . It is due to the proton transfer reaction that leads to the formation of nitric acid. S elf catalytic decomposition reaction of the ionic solution then occurs in the vicinity of the electrode with existence of excess nitric acid , and brownish nitrogen oxides gas is emitted from the liquid . Experiments have shown that the nitrogen oxides in the product ga s of decompositi on depends on voltages and pressures, which further confirm that the liquid phase electrochemical reaction s are essential to the decomposition process. T h e findings lay the foundation for future designs of a electrolytic ignition module for HAN based prope llants.

Paper ID: P1302

Catalytic decomposition of HAN-based monopropellants with hexaaluminates

Kuan-Io Lao (National Cheng Kung University), Yan-Ze Song (National Cheng Kung University), Ming-Hsun Wu (National Cheng Kung University)

The purpose of this study is to investigate the catalytic performance of LaMn-hexaaluminates catalysts on hydroxylammonia nitrate (HAN) aqueous solution under pressures relevant to space propulsion applications. HAN is a promising “green” liquid monopropellantthat can potentially replace the widely-used, but highly toxic space propellant, hydrazine. But due to the relatively high reaction temperature and acidity of HAN, the existing catalysts for hydrazine may not be suitable for HAN propellants. Hexaaluminates, which have demonstrated good sustainability in high temperature applications, is an interesting option for the ignition of HAN-based propellants. Experiments were conducted using a high-pressure vessel equipped with a heating block on the bottom that holds the sample crucible. Hexaaluminate catalyst was placed in the crucible with 76 wt.% HAN aqueous solution, and being heated from 30 ℃ to 235 ℃ at 12.5 ℃/min. The vessel was filled with Aegon, and the test pressure ranges from 0.1 to 3.1 MPa. Gas analysis was also carried out to quantify decomposition product species including NO, N_2O, and NO_2. The results show that all the catalysts tested are able to reduce the decomposition onset temperature, shorten the reaction time as well as induction time. Product gas analyses further shows that reaction completeness is enhanced with catalytic decomposition comparing to thermal decomposition. It is worth noting that with the existence of LaMn-hexaaaluminate catalysts, the linear burning rate of HAN solutions becomes less pressure dependent.

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