



CCE News

# **Center for Combustion Energy**





**Education** 



http://www.cce.tsinghua.edu.cn/

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# **Message from the Director**





*Cover page picture credit: Jialong Huo, graduate student.* 

being a minor participant of singledigit number of presentations to the second largest sectional entity in the number of presentations at a symposium. The above observation puts in a nutshell the potential contributions that could further result from the empowerment of such a large sector of the international scientific community in combustion. The CCE is proud to be part of this spectacular rise in scientific activity!

The CCE was established with the singular goal of becoming an internationally prominent research and education body in combustion, with an agenda of core research that comprises foundation science, energy science, and interdisciplinary science, as shown in the chart below. This is a tall order, a goal that we have been striving to accomplish through the recruitment of firstrate researchers, as well as the support of Tsinghua University and our colleagues in China and internationally.

The goal of talent recruitment



has been particularly challenging. We are therefore immensely gratified to have assembled an outstanding group of faculty who are both front-rank researchers and also dedicated teachers. Their research accomplishments and professional stature are evidenced by having been selected for the coveted 1000 Talent Award (3 in total) and 1000 Young Talent Award (7), administered by the Chinese government, and appointments (5) to the editorial boards of front-rank journals. These colleagues, almost entirely recruited from overseas and brimming with enthusiasm and confidence, basically hit the ground and started running upon joining the Center. The charge that they are given is simply to do the best science that they know how, with the aspiration that in due time each of them will evolve into a major international figure of prominence in his/her area of endeavor. The upward trajectory that they have so far mapped has been impressive, with significant research results



steadily coming out and published in leading journals. Some of the ongoing research, together with a list of recent journal articles, is reported in this issue.

The Center now has about 60 doctoral students, with the goal of reaching 100 in steady operation. We have also sent some of them for short-term visits to colleagues overseas for enrichment and collaboration, from three months to a year. Since these students are already well trained in their knowledge and skill, such visits have been particularly fruitful to both us and the hosts, invariably leading to joint publications and long-term collaboration.

In terms of outreach, perhaps our signature accomplishment is the offering of the annual summer school on combustion, starting from 2012. This summer school, patterned after the highly successful Princeton Summer School, routinely attracted about 400 participants from China as well as internationally. A rich and intense week-long academic program is conducted by worldleading authorities who are known



as both powerful researchers and inspirational instructors. We are pleased with the catalyzing role that this summer school series has played in the rapid increase in high-level combustion research and networking activities in China in recent years.

We hope to communicate the exciting developments at the CCE through this newsletter series to the international combustion and energy community at regular intervals, currently aiming biannually. Since this is the first issue subsequent to our founding a few years ago, in this and several future issues we shall also report some relevant items developed during this interim period.

I end this message by thanking all our friends, in China and internationally, for your collegial support of our growth in the past years in so many ways. In return, we at the CCE pledge our dedication to working with you in the advancement of combustion and the betterment of humanity. Together we shall make a difference.

Chang K. Law

Chung K. Law 2018.01.01



# Research

# **Program Overview**

We strive to conduct leading-edge fundamental research in combustion, fluids and energy science, with strong emphasis on practical relevance and interdisciplinary synergy. To date, we have developed strong programs in the following areas, with potential applications in power generation, energy technology, propulsion, emission control, and fire/explosion safety.

- Fluid Mechanics: Turbulent and Two-Phase Flows
- Laminar and Turbulent Combustion
- Combustion Chemical Kinetics
- Detonation Phenomena
- Combustion Emission and Environmental Impact
- Microgravity and Space Science
- Diagnostics for Combustion and Turbulent Flows



The Good, the Bad, the Ugly: To demonstrate the intellectual richness and aesthetic beauty of combustion phenomena, these are three possible modes of spark-ignited flame propagation and morphology in hydrogen-air mixtures. From left to right: rich mixture and quiescent environment, showing a smooth expanding front (similar to the image on the cover); lean mixture and quiescent environment, showing flame-front wrinkling by intrinsic cellular instability; any mixture in turbulent environment, showing flame-front wrinkling by imposed turbulent eddies. These images, contributed by Professor C.K. Law and his associates at Princeton University, won the First Place Award of Combustion Art Competition at the 8th US National Combustion Meeting.



# The Research Team

#### Fluids + Chemistry



Chung K. Law Founded CCE in 2010 Ph. D., (1973) University of California-San Diego



Zhuyin Ren Joined CCE in 2013 Ph. D., (2006) Cornell University



Kai H. Luo Joined CCE in 2011 Ph. D., (1992) University of Cambridge



Damir Valiev Joined CCE in 2016 Ph. D., (2008) Royal Institute of Technology

#### **Combustion Kinetics**



Xiaoqing You Joined CCE in 2011 Ph. D., (2008)

University of Southern California



Xuefei Xu Joined CCE in 2015 Ph. D., (2006) Xiamen University



Bin Yang Joined CCE in 2012 Ph. D., (2006) University of Science and Technology of China



Rémy Mével Joined CCE in 2017 Ph. D., (2009) University of Orléans

#### Interdisciplinary



Suyuan Yu Joined CCE in 2013 Ph. D., (1998) University of California-Davis (Thermal and nuclear science)



Yu-Cheng Liu Joined CCE in 2016 Ph. D., (2013) Cornell University (Low- and super-gravity combustion)

#### **Fluid Mechanics**



Haitao Xu Joined CCE in 2014 Ph. D., (2003) Cornell University



Chao Sun Joined CCE in 2015 Ph. D., (2006) Chinese University of Hong Kong

#### Instrumentation



Xing Chao Joined CCE in 2015 Ph. D., (2013) Stanford University



# **Research Highlights**



Xiaoqing You is currently an associate professor at the CCE and the Department of Energy and Power Engineering, working in the field of combustion kinetics. Her present research focuses on the following four topics: 1) key elementary reactions in fuel combustion using a combination of electronic structure calculations and reaction rate theories; 2) kinetic model development for fuel combustion and pollutant formation; 3) reaction kinetics of soot nucleation, surface growth and oxidation; 4) experimental and modeling studies of nascent soot formation.

# **Mechanism of Soot Formation**

Air pollution by fine particles, especially ultrafine particulate matter (PM2.5, i.e. aerodynamic diameter  $\leq 2.5 \ \mu$  m), has become one of the most serious environmental problems in China, posing serious threat to human health. While the formation of PM2.5 is very complex, a major source is fossil fuel combustion. As fossil fuels remain to be the primary energy sources, PM2.5 continues to be an important air pollutant. To reduce air pollution, it is essential to control emissions through optimal design of fuels and engines, which requires a fundamental understanding of the mechanism of particle formation.

Prof. You and her research team are interested in understanding the formation of condensed-phase carbon materials, i.e. soot, from reacting gases. Supported by the National Science Foundation of China and the National Basic Research Program, Prof. You's research team has made much progress in exploring the mechanism of soot formation both theoretically and experimentally in recent few years. In view of the multi-radical characteristics of certain polycyclic aromatic hydrocarbons (PAHs), they explored new possible reaction paths of soot nucleation and soot surface growth. Their study demonstrates that localized  $\pi$  electrons in PAHs promote the formation of stable PAH dimers (Journal of Physical Chemistry A, 2014, 118:1287). Similar to the PAHs, the multi-radical characteristics of the local structure of soot surface facilitate the addition of unsaturated aliphatics. This new growth path explains the experimental observations of soot mass growth in low-temperature post-flame region that could not be explained by previous theories (Journal of Physical Chemistry Letters, 2015, 6:477 and Journal of Physical Chemistry A, 2016, 120:683). Furthermore, they have studied the kinetics of thermal decomposition of graphene oxyradicals, an important reaction during soot surface oxidation, and discussed the ways of determining effective rate coefficients for cases where the collisional relaxation rate competes with the dissociation rate (Physical Chemistry Chemical

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*Physics*, 2016, 18:12149, and 2017, 19:11064).

Experimentally, Prof. You's group has built a laminar premixed burner-stabilized stagnation flame for studying the mobility size down to ~1 nm of nascent soot particles for both gaseous and liquid fuel combustion (Combustion and Flame, 2015, 162:3810, 2016, 165:424, and 2018, 187: 239, and *Proceedings of the Combustion Institute*, 2017, 36:993). In addition, they are studying particle formation under constant temperature condition in a heated flow reactor, so that the characteristics of nascent soot over a wide range of temperatures (1200-1800 K) can be established.





Chao Sun obtained his PhD from the Chinese University of Hong Kong in 2006, and received the Hong Kong Young Scientist award in the same year. In 2015, he joined the Center of Combustion Energy and Department of Energy and Power Engineering at Tsinghua University as a Full Professor and was selected by the Thousand Talents Program. Prof. Sun's research interests include high-Reynolds number turbulence, bubbles and drops, multiphase flows, heat and mass transfer, and microfluidics.

# Multiphase flow and Turbulence: Rising particles through fluids and controlling turbulent flow using ratchet surfaces

# 1. Rotation triggers the zig-zag of buoyant particles rising through fluids

It is somewhat puzzling that a heavy object sinks straight in water, while a buoyant air-bubble or a balloon zig-zags or spirals while rising through water. This observation has been famously coined as "Leonardo' s paradox". A popular explanation has been proposed: that the mass (or weight) of the rising or falling body governs its path-oscillations, and when the body becomes buoyant, it starts to oscillate vigorously.

Recently, researchers at University of Twente and the CCE have revealed that it is not the mass of the body, but instead, mainly its moment of inertia that causes a rising particle or air bubble to zig-zag. They uncover the various kinds of path-and wake-instabilities



that result for freely rising/falling particles in still fluid. The results are supplemented by predictions for the existence of two regimes of motion and wake-transitions, all induced by moment of inertia change. These results will have strong bearing on our understanding of everyday observations, for example: on the zig-zag paths of air bubbles rising in an aquarium tank. It is likely that the underlying rotation of the rising bubble causes it to zig-zag or spiral.

**Reference:** V. Mathai, X. Zhu, C. Sun, and D. Lohse, *Physical Review Letters* (119,054501, 2017).

# 2. Controlling turbulent flow using ratchet surfaces

Turbulent flows over rough surfaces are ubiquitous in engineering and geophysical flows. Examples include convective flows in the atmosphere and in oceans, where the ground, sea-bed and ocean floor are generally not smooth. The vast majority of the studies with rough walls adopt some ordered and



Wake transitions for rising cylinders. From (A) to (D), the 2S wake mode transitions to 2P wake mode.

symmetrical structures, such as pyramids, squares, rectangles etc. However, the rough surfaces in engineering applications and in nature are in general not symmetric, resulting in complex interactions between the flow and the asymmetric roughness elements. Examples are wind blowing over a landscape with asymmetric slopes and ocean flows over an asymmetric sea-bed, etc. Other examples include marine animals which can actively change the asymmetric roughness for maneuverability.

Drawing inspiration from the classical Feynman-Smoluchowski ratchet, researchers from the CCE, Hechuan Jiang et al., University of Twente and University of Rome "Tor Vergata" studied the influences of ratchet-like wall structures on the flow organization and heat transfer in fully developed convective thermal turbulence. They find that the turbulent flow has a preferred direction due to the broken symmetry of the system and meanwhile can be controlled. The findings provide many flow control opportunities to achieve stable flow structures with desirable transport efficiencies. They are also relevant to oceanic and geo-physical scenarios, such as wind blowing over a landscape with asymmetric slopes and ocean flows over an asymmetric sea-bed, etc.

Reference: H. Jiang, X. Zhu, V. Mathai, R. Verzicco, D. Lohse, and C. Sun, *Physical Review Letters*, 2018, 120, 044501.





Xu Xuefei received her Ph.D. in 2006, from the Department of Chemistry at Xiamen University. In 2015, Dr. Xu was selected by the national "1000 Young Talents program" and joined CCE and the Department of Energy and Power Engineering as an associate professor University. Her research interests include theoretical and computational study of photochemistry, atmospheric chemistry, combustion chemistry, and kinetics.

# Kinetics of the Methanol Reaction with OH at Interstellar, Atmospheric, and Combustion Temperatures

The reaction of OH with methanol has received much attention by combustion chemists, atmospheric scientists, and astrophysical chemists for its importance over a broad temperature range. In 2013, Shannon et al. (*Nat. Chem.* 2013, 5, 745) reported a surprisingly large rate coefficient at 82 and 63 K and an unexpectedly large negative temperature dependence (NTD) of the rate constant below 200 K, and they attributed the mechanism to tunneling through the barrier via a long-lived hydrogen-bonded pre-reactive complex at low temperatures.

For understanding the reaction better, recently, the researchers from the CCE, the University of Minnesota, Gaussian Inc. and Universidade de Santiago de Compostela employed the competitive canonical unified statistical (CCUS) model in both high-pressure and low-pressure limits to do a unified treatment of this reaction that spans the broad temperature range encompassing the interstellar, atmospheric, and combustion regimes.

They found a significant effect of the anharmonicity of high-frequency modes of transition states on the low-temperature rate constant, and showed how tunneling leads to an unusual negative temperature dependence of the



The total rate constants in the low-pressure-limit (LPL) and the highpressure-limit (HPL).



rate constants in the range 200 K > T > 100 K. The calculations also demonstrate the importance of the extent of stabilization of the pre-reactive complex. The capture rate for the formation of the complex is the dominant dynamical bottleneck for T < 100 K, and it leads to weak temperature dependence of the rate below 100 K in the high-pressure-limit of the CCUS model. They also reported the

pressure dependence of the branching ratios and the kinetic isotope effects (KIEs), and an unusual nonmonotonic variation of the KIE in the highpressure limit at low temperatures.

**Reference:** Lu Gem Gao, Jingjing Zheng, Antonio Fernández-Ramos, Donald G. Truhlar, and Xuefei Xu, *J. Am. Chem. Soc.*, 2018, 140, 2906 2918.



Chung K. Law is the Robert H. Goddard of Princeton University and the founding director of the CCE. His research interests are in combustion, propulsion, heat and mass transfer, energy, alternative fuels and the environment. He is a member of the US National Academy of Engineering (NAE), a fellow of several professional organizations including the American Academy of Arts and Sciences (AAAS), a former president of the Combustion Institute, and the recipient of a number of honorific professional awards.

# Analytical Description of Explosion Limits of Hydrogen-Oxygen Mixtures

Combustion phenomena are frequently characterized by complex chemical kinetics that resist analyticity in their description. By using the intrinsically nonmonotonic, chain-dominated explosion limits of hydrogen-oxygen mixtures as an example, we propose herein a formulation that holds potential for further development. Specifically, in the pressure– temperature space (Fig. 1), the transition boundary for explosivity shows a Z-shaped curve that consists of three explosion limits such that at low and high temperatures, the mixture transitions from nonexplosive to explosive states with increasing pressure. However, within an intermediate temperature range, with increasing pressure the mixture will traverse a sequence of nonexplosive, explosive, nonexplosive and explosive states. This behavior is the consequence of gas-phase chain branching competing with the loss mechanisms of gas-phase chain termination and wall destruction.

Our formulation has proceeded in two stages. First, by ignoring the radical-radical reactions relevant at high pressures, the chemical system was linearized and analyzed [1]. By further letting H and HO<sub>2</sub> to





be the only unsteady species, the explosion limits were found to be governed by a cubic equation in terms of the system pressure, with the three explosion limits corresponding to its three distinct roots. The analytical result also led to the derivation of the separate singlelimit and double-limit expressions, as well as the critical condition that the explosion limits lose their nonmonotonicity.

The second step [2] includes the radical-radical reactions involving the HO<sub>2</sub> and  $H_2O_2$  reactions, which render the chemical system nonlinear. The problem was subsequently solved using the homotopic perturbation method, leading to an accurate analytical expression

describing the entire explosion Z-curve.

This collaborative study between the CCE and Princeton University lays the groundwork for further analytical studies of combustion systems characterized by complex reaction mechanisms, while at the same time it yields an accurate analytic solution for an important combustion problem.

#### **Reference:**

[1] Xianming Wang, Chung K. Law, An analysis of the explosion limits of hydrogen-oxygen mixtures, *J. Chem. Phys.*, 138, 134305 (2013).

[2] Wenkai Liang, Chung K. Law, An analysis of the explosion limits of hydrogen/oxygen mixtures with nonlinear chain reactions, *Phys. Chem. Chem. Phys.*, 20, 742-751 (2018). \*\*Cover Article and 2017 PCCP Hot article\*\*



Figure 1. Explosion limits of a stoichiometric hydrogen-oxygen mixture



## **Graduate Student Presentation**



Wenyu Sun is from Hubei Province and obtained her bachelor degree from Huazhong University of Science and Technology. She joined the CCE in 2013 and is advised by Prof. Bin Yang.

Wenyu Sun's research projects are on the combustion kinetics of oxygenated fuels which represent promising alternatives to traditional fossil fuels. In order to build and validate detailed kinetic models for oxygenated fuels, attention is brought on: (i) exploring how the chemical functionalities of the fuel affect the combustion characteristics; (ii) revealing the role of specific reaction class in different temperature and pressure regimes; and (iii) elucidating the effects of oxygenated alternatives on pollutant formation. Wenyu has reported her results in eight journal articles in *Combustion and Flame* and *Proceedings of* 



Qian Mao is from Zhejiang Province and graduated from the Department of Energy and Power Engineering at Shandong University. She joined the center in 2013 and is advised by Prof. Kaihong Luo.

Qian Mao's research projects are on the application of molecular dynamics simulation to the formation, dynamics, and chemical properties of nanomaterials. She has studied the collision and coalescence of titanium oxide nanoparticles as well as the phase transformation induced by the sintering of these particles. She investigated the nucleation mechanism of soot particles formed under combustion relevant conditions. She also examined the catalytic combustion of methane on palladium/palladium oxide metal clusters. Qian has published five first-authored



functionalities, affect combustion characteristics;the role of specific reaction class in different temperature and

pressure regimes;

the effects of oxygenated alternatives addition on pollutants formation.

*the Combustion Institute*, including five as a first author. She received the Best Presentation Award in the CCE for the year 2016.

journal articles in *Carbon*, *Proceedings of the Combustion Institute, Journal of Physical Chemistry C* etc. Qian received an Outstanding Paper Award at the China National Symposium on Combustion in 2016.



Time evolution of the number of the crystal atom of  $\text{TiO}_2$ polymorphs in the last sintering stage of two equal-sized 2.5 nm particles at  $T_0 = 1473$  K.



# **Scientific Production**

The number of faculty has now reached thirteen with six new members joining within the last two years. The number of graduate students is continuously increasing with sixteen new students joining the center last September, bringing the total number to 59. More than 200 ISI journal articles have been published over the past six years in premier scientific journals such as *Combustion and Flame, Journal of Fluid Mechanics, Journal of Physical Chemistry Letters, Physical Review Letters, Proceedings of the Combustion Institute,* and *Progress in Energy and Combustion Science.* 



# List of ISI Journal Articles Published in 2017 by Members of the Center for Combustion Energy

55) L.R. Boeck, M. Meijers, A. Kink, R. Mevel, J.E. Shepherd: "Ignition of fuel-air mixtures from a hot circular cylinder", *Combustion and Flame*, 2017, vol 185, p 265-277.

54) W.Y. Sun, T. Tao, R.Z. Zhang, H.D. Liao, C. Huang, F. Zhang, X.Y. Zhang, Y. Zhang, B. Yang: "Experimental and modeling efforts towards a better understanding of the high-temperature combustion kinetics of C3-C5 ethylesters", *Combustion and Flame*, 2017, vol 185, p 173-187.

53) L.Y. Jing, X.Q. You, J.L. Huo, M. Zhu, and Z.P. Yao: "Experimental and numerical studies of ammonium dinitramide based liquid propellant combustion in space thruster", *Aerospace Science and Technology*, 2017, vol 69, pp. 161-170.

52) T.Q. Zhang, S.Y. Yu, W. Peng, Q. Sun, Y.Y. Jiang, and Q. Shi: "Resuspension of multilayer graphite dust particles in a high temperature gascooled reactor", *Nuclear Engineering and Design*, 2017, vol 322, p 497-503.

51) C. Huang, B. Yang, and F. Zhang: "Initiation mechanism of 1,3-butadiene combustion and its effect on soot precursors", *Combustion and Flame*, 2017, vol 184, p 167-175.

50) L.R. Boeck, R. Mevel and T. Sattelmayer: "Models for shock-induced ignition evaluated by detailed chemical kinetics for hydrogen/air in the context of deflagration-to-detonation transition", *Journal of Loss Prevention in the Process Industries*, 2017, vol 49, p 731-738.

49) S.B. Wang, Y.C. Wu, R. Miao, M.W. Zhang, X.X. Lu, B. Zhang, A. Kinstler, Z.Y. Ren, Y.B. Guo, and T.F. Lu: "Scalable continuous flow synthesis of Zno nanorod arrays in 3-D ceramic honeycomb substrate for low temperature desulfurization", *CrystEngComm*, 2017, vol 19, p 5128-5136.



48) D. Christopher, P.X. Jiang, and X. Zhang: "Editorial: Special Issue for the 9th International Symposium on Heat Transfer in Beijing", *Applied Thermal Engineering*, 2017, vol 124, p 44.

47) P. Zhang, S. Li, Y.D. Wang, W.Q. Ji, W.Y. Sun, B. Yang, X. He, Z. Wang, C.K. Law, and F. Zhang: "Measurement of reaction rate constants using RCM: A case study of decomposition of dimethylcarbonate to dimethyl ether", *Combustion and Flame*, 2017, vol 183, p 30-38.

46) Q. Mao, A.C.T. van Duin, and K.H. Luo: "Formation of incipient soot particles from polycyclic aromatic hydrocarbons: A ReaxFF molecular dynamics study", *Carbon*, 2017, vol 121, p 380-388.

45) E. Almeras, V. Mathai, D. Lohse, and C. Sun: "Experimental investigation of the turbulence induced by a bubble swarm rising within incident turbulence", *Journal of Fluid Mechanics*, 2017, vol 825, p 1091-1112

44) V. Mathai, X.J. Zhu, C. Sun, and D. Lohse: "Mass and moment of inertia govern the transition in the dynamics and wakes of freely rising and falling cylinders", *Physical Review Letters*, 207, vol 119(5), 054501.

43) P.B.J. Hoefnagels, P. Wei, D.N. Guzman, C. Sun, D. Lohse, and G. Ahlers: "Large-scale flow and Reynolds numbers in the presence of boiling in locally heated turbulent convection", *Physical Review Fluids*, 2017, vol 2(7), 074604.

42) X.Y. Li, X.Q. You, C.K. Law, and D.G. Truhlar: "Kinetics and branching fractions of the hydrogen abstraction reaction from methyl butenoates by H atoms", *Physical Chemistry Chemical Physics*, 2017, vol 19(25), p 16563-16575. 41) H. Zhou, S. Li, Z. Ren, and D.H. Rowinski: "Investigation of mixing model performance in transported PDF calculations of turbulent lean premixed jet flames through Lagrangian statistics and sensitivity analysis", *Combustion and Flame*, 2017, vol 181, p 136-148.

40) Z. Wang, H. Liu, and R.D. Reitz: "Knocking combustion in spark-ignition engines", *Progress in Energy and Combustion Science*, 2017, vol 61, p 78-112.

39) H.J. Guo, H.C. Ding, Y.F. Li, X. Ma, Z. Wang, H.M. Xu, and J.X. Wang: "Comparison of spray collapses at elevated ambient pressure and flash boiling conditions using multi-hole gasoline direct injector", *Fuel*, 2017, vol 199, p 125-134.

38) W.Y. Sun, C. Huang, T. Tao, F. Zhang, W. Li, N. Hansen, and B. Yang: "Exploring the high-temperature kinetics of diethyl carbonate (DEC) under pyrolysis and flame conditions", *Combustion and Flame*, 2017, vol 181, p 71-81.

37) C. Huang, B. Yang, and F. Zhang: "Pressure-dependent kinetics on the  $C_4H_7$  potential energy surface and its effect on combustion kinetic model predictions", *Combustion and Flame*, 2017, vol 181, p 100-109.

36) N. Hansen, R.S. Tranter, K. Moshammer, J.B. Randazzo, J.P.A. Lockhart, P.G. Fugazzi, T. Tao, and A.L. Kastergren: "2D-imaging of sampling-probe perturbations in laminar premixed flames using Kr X-ray fluorescence", *Combustion and Flame*, 2017, vol 181, p 214-224.

35) T.Q. Zhang, S.Y. Yu, Q. Sun, W. Peng, and J. Wang: "Study on the resuspension of graphite dust based on the Rock' n' Roll model", *Progress in Nuclear Energy*, 2017, vol 98, p 313-320.

34) G.Z. Xing, Y.B. Zhao, M. Modestov, C. Zhou, Y. Gao, and C.K. Law: "Thermal-diffusional instability in white dwarf flames: Regimes of flame pulsation", *The Astrophysical Journal*, 2017, vol 841(1), 21.

33) H.M. Wang, X.Q. You, M.A. Blitz, M.J. Pilling, and S.H. Robertson: "Obtaining effective rate coefficients to describe the decomposition kinetics of the corannulene oxyradical at high temperatures", *Physical Chemistry Chemical Physics*, 2017, vol 19(18), p 11064-11074.



32) M. Shirota, M.A.J. van Limbeek, D. Lohse, and C. Sun: "Measuring thin films using quantitative frustrated total internal reflection (FTIR)", *The European Physical Journal E*, 2017, vol 40(5), p 1-9.

31) W. Peng, T. Chen, Q. Sun, J. Wang, and S.Y. Yu: "Preliminary experiment design of graphite dust emission measurement under accident conditions for HTGR", *Nuclear Engineering and Design*, 2017, vol 316, p 218-227.

30) Z. Lu, H. Zhou, S. Li, Z.Y. Ren, T.F. Lu, and C.K. Law: "Analysis of operator splitting errors for near-limit flame simulations", *Journal of Computational Physics*, 2017, vol 335(15), p 578-591.

29) S. Li, H. Zhou, L.Y. Hou, and Z. Ren: "An analytic model for the effects of nitrogen dilution and premixing characteristics on NOx formation in turbulent premixed hydrogen flames", *International Journal of Hydrogen Energy*, 2017, vol 42(10), p 7060-7070.

28) J. Luo, R. Pohl, L.H. Qi, G.W. Romer, C. Sun, D. Lohse, and C.W. Visser: "Printing functional 3D microdevices by laser-induced forward transfer", *Small*, 2017, vol 13(9), 1602553.

27) R. Meana-Paneda, X.F. Xu, H. Ma, and D.G. Truhlar: "Computational kinetics by variational transition-state theory with semiclassical multidimentional tunneling: direct dynamics rate constants for the abstraction of H from CH<sub>3</sub>OH by triplet oxygen atoms", *The Journal of Physical Chemistry A*, 2017, vol 121(1), p 1693-1707

26) Y. Gao, and Y.Q. Lou: "Variable protostellar mass accretion rates in cloud cores", *Monthly Notice of the Royal Astronomical Society Letters*, 2017, vol 466, p L53-L57.

25) M. Kuron, Z.Y. Ren, E.R. Hawkes, H. Zhou, H. Kolla, J.H. Chen, and T.F. Lu: "A mixing timescale model for TPDF simulations of turbulent premixed flames", *Combustion and Flame*, 2017, vol 177, p 171-183.

24) T. Yao, Y.J. Pei, B.J. Zhong, S. Som, T.F. Lu, and K.H. Luo: "A compact skeletal mechanism for n-dodecane with optimized semi-global low-temperature chemistry for diesel engine simulations", *Fuel*, 2017, vol 191, p 339-349.

23) Y. Zhang, Q. Zhou, and C. Sun: "Statistics of kinetic and thermal energy dissipation rates in two-dimensional turbulent Rayleigh-Benard convection", *Journal of Fluid Mechanics*, 2017, vol 814, p 165-184.

22) L. Jing, J.L. Huo, H.M. Wang, X.Q. You, M. Zhu, Y.M. Yang, and Z.P. Yao: "Experimental investigation on the evaporation and combustion processes of ammonium-dinitramide-based liquid propellant", *Journal of Propulsion and Power, 2017*, vol 33(2), p 343-349.

21) S. Wildeman, S. Sterl, C. Sun, and D. Lohse: "Fast dynamics of water droplets freezing from the outside in", *Physical Review Letters*, 2017, vol 118(8), 084101.

20) H.J. Guo, X. Ma, Y.F. Li, S. Liang, Z. Wang, H.M. Xu, and J.X. Wang: "Effect of flash boiling on microscopic and macroscopic spray characteristics in optical GDI engine". *Fuel*, 2017, vol 190, p 79-89.

19) W.H. Han, Y. Gao, and C.K. Law: "Flame acceleration and deflagration- to-detonation transition in micro- and macro-channels: An integrated mechanistic study", *Combustion and Flame*, 2017, vol 176, p 285-298.

18) W.H. Han, W.J. Kong, Y. Gao, and C.K. Law: "The role of global curvature on the structure and propagation of weakly unstable cylindrical detonations", *Journal of Fluid Mechanics*, 2017, vol 813, p 458-481.

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and modeling study", Proceedings of the Combustion Institute, 2017, vol 36, p 1269-1278.

15) M. Kuron, E.R. Hawkes, Z.Y. Ren, J.C.K. Tang, H. Zhou, J.H. Chen, and T.F. Lu: "Performance of transported PDF mixing models in a turbulent premixed flame", *Proceedings of the Combustion Institute*, 2017, vol 36(2), p 1987-1995.
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The full list for 2011-2017 is available on CCE website: http://www.cce.tsinghua.edu.cn/en

## Academic Programs

The CCE offers both undergraduate and graduate academic programs, which are briefly described in this section.

# Undergraduate program

The undergraduate course of study is conducted under the Advanced Clean Energy (ACE) academic program. Tsinghua University emphasizes international teaching and research. The pedagogical system and the curriculum design of the ACE program refers to the successful experience of engineering disciplines in world-class universities such as Princeton, UC-Berkeley, Stanford, MIT, Caltech, Cornell, etc. It aims at nurturing academic and professional leadership talents with a broad foundation



Prof. M. Louge from Cornell University teaching thermodynamics to the ACE 2016 class

of fundamental knowledge, innovative and critical thinking, appreciation of practice, an international outlook, and having the personality and aspiration to serve humanity in general and the country in particular. Visiting faculties who are well known as master teachers will give guest lectures and courses.

The academic program is four years. A flexible duration of learning is adopted based on a credit management system. Completion of the ACE program leads to the conferral of the Bachelor of Science in Engineering from one of the Department of Energy and Power Engineering, the Department of Automotive Engineering, and the School of Aerospace Engineering. The ACE program was started in 2015, with a class of 23 competitively selected outstanding freshmen students. The class of 2016 is also composed of 23 students.

# Graduate program

The graduate program aims to empower its graduates with a broad knowledge of combustion science and technology; the expertise in the specific area of the thesis research; the ability to exercise critical thinking and to appreciate scientific beauty, and a passion





of lifelong learning. The graduates are expected to assume leadership positions in scientific communities and the society at large, with honorable and high ethical standards, passion for knowledge discovery, and compassion for humanity.

The Center courses are conducted in English, given by our faculty who are almost entirely recruited from leading institutions in the U.S. and Europe. Students have the opportunities to meet world leading experts in fluids and combustion through invited seminars and other outreach activities such as the Tsinghua-Princeton Summer School on Combustion. Through their participation in our wellfunded projects in the areas of aero-engine combustion, combustion chemical kinetics, multi-phase flows, turbulent flows, and diagnostics, they are nurtured to possess skills to conduct forefront, discovery-level research based on the most fundamental and rigorous elements of experiment, theory, and numerical simulation. Short-term visits of three months to a year to colleagues overseas for enrichment and collaboration research can also be arranged.



ACE class of 2015



ACE class of 2016



## **Organization and History**

The goal and algorithm of the Tsinghua Summer School on Combustion is modeled after the highly successful Princeton Summer School on Combustion. It is organized by Tsinghua University, endorsed by the Chinese Section of the Combustion Institute, and recently co-sponsored by the Combustion Institute. It has been extensively attended by members of the Chinese section as well as other Asian and international regional sections.

The Summer School was inaugurated in 2012 and has since been held annually. Every year, close to 400 participants attended the courses given by worldrenowned combustion experts. Apart from the courses, career panel discussion, laboratory tour, topical discussion sessions and posters sessions have also been organized.

The Tsinghua Summer School has become an important enrichment and outreach program for education of the next generation combustion scientists in China. It has attracted immense interest and enthusiastic participation not only from academia but also industrial and research entities. Furthermore, similar to the experience of the Princeton Summer School, the Tsinghua Summer School provides an excellent platform for networking among young scientists from different universities, industries and geographical locations. Detailed information can be found on the CCE website.

# 2017 Summer School

For the 2017 session, 380 attendees joined the Summer School during which five courses were given by a team of highly effective lecturers:



**Ronald K. Hanson** taught Quantitative Laser Diagnostics for Combustion Chemistry and Propulsion. Prof. Hanson is the Woodard Professor of Mechanical

Engineering at Stanford University. He received his Ph.D. from Stanford and chairs the international advisory committee of the CCE University in 1968. He is a Fellow of the American Institute of Aeronautics and Astronautics (AIAA), the American Society of Mechanical Engineers (ASME) and the Optical Society of America (OSA), and is a member of the US National Academy of Engineering (NAE).



**Michael J. Pilling** taught the Combustion Chemistry course. Prof. Pilling is Professor of Physical Chemistry at Leeds University in UK since 1989. He received



his Ph.D. from Cambridge University in 1967. His research focuses on fundamental chemical kinetics and applications in atmospheric chemistry and combustion. He has published over 300 papers and has received a number of awards, including a CBE in 2008.



Thierry Poinsot taught the Computational Turbulent Combustion course. Dr. Poinsot is the Research Director at the Institut de Mécanique des Fluides

of Toulouse in France, as well as head of the CFD group at CERFACS and senior research fellow at Stanford University. His research interests are in combustion theory, models and numerical methods for turbulent and laminar flames, combustion instabilities, massively parallel simulations for gas turbines, piston engines, rockets and furnaces.



**Heinz Pitsch** taught the Combustion Theory course. Prof. Pitsch is the Director of the Institute for Combustion Technology at Aachen University. He received his Ph.D. in mechanical engineering from Aachen University in 1998. His main research interests are in the fields of combustion theory, combustion chemistry, turbulence, turbulent combustion, and multi-phase flows with application to technical combustion systems. He is a co-chair for the upcoming 37<sup>th</sup> International Combustion Symposium.



**Richard A. Yetter** taught Combustion of Energetic Materials. Prof. Yetter is Professor of Mechanical Engineering at the Pennsylvania State University. He received his PhD from Princeton

University. His research interests encompass high temperature combustion chemistry, heterogeneous combustion, and energetic materials. Prof. Yetter is the Editor-in-Chief of *Combustion Science and Technology.* 





## 2018 Summer School Announcement

## TSINGHUA - PRINCETON -COMBUSTION INSTITUTE



The technical program for the 2018 Summer School has been formulated, as follows:

#### **Combustion Theory**

Lecturer: Prof. **Moshe Matalon**, University of Illinois at Urbana-Champaign, USA

#### **Combustion Chemistry and Modeling**

Lecturer: Prof. **Henry J. Curran**, National University of Ireland, Ireland

Turbulent Combustion : Modelling and Applications Lecturer: Prof. Epaminondas Mastorakos, University of Cambridge, UK Laser Diagnostic in Turbulent Combustion Research Lecturer: Prof. Jeffrey A. Sutton, Ohio State University, USA

We are most grateful to the lecturers, who have accepted our invitation to undertake the extremely demanding task of preparing and delivering their respective courses. On behalf of the community, and especially all the participants, we thank them in advance.

The Summer School will be held at Tsinghua University. On-campus dormitory and hotel lodging, as well as meal plans covering breakfast, lunch and dinner, will be available to all participants. Specifically, lecture rooms will be classrooms with modern facilities; campus hotels at different levels will be blocked for students and senior participants, with private bathrooms and air conditioning; meals will be provided in various campus canteens and restaurants. There is also a large selection of hotels and restaurants around the campus.

#### **Further Inquiries**

Direct inquiries on the 2018 Summer School on the academic program and the logistics of participation to either the program administrator, Ms. Hong Tian, (86)10-62796768, ccess@tsinghua.edu.cn, or the program co-organizer, Dr. Yu-Cheng Liu, <u>ycliu7@</u> <u>mail.tsinghua.edu.cn</u>



# Group Pictures of the Summer School Participants (2012-2017)















# News

## Prof. C.K. Law Received the Beijing Great Wall Friendship Award

Prof. C.K. Law received the Beijing Great Wall Friendship Award from the Beijing Municipal Government on Sept. 29, 2017. This prize is the highest distinction presented by the Beijing Municipal Government. It was established in 1999 to honor notable foreign experts for their outstanding contributions to the city's development.



Prof. C.K. Law receiving the Friendship Award



Hua Zhou and other winners with their award certificates

## CCE Student Hua Zhou Won Young Investigator Award at the 11<sup>th</sup> Asian-Pacific Conference on Combustion

At the 11th Asian-Pacific Conference on Combustion, Hua Zhou received a Young Investigator Award for his paper entitled "RANS-PDF Simulations of Piloted Premixed Jet Flames", presented at the 10th Conference. Hua is co-advised by Profs. C.K. Law and Zhuyin Ren.

Prof. Xiaoqing You and her students, Q.X. Tang, B.Q. Ge and Q. Ni, received the Outstanding Paper Award at the 2017 Annual Conference of the Chinese Society of Engineering Thermophysics on Combustion for their paper ``Soot formation characteristics of n-heptane/ toluene mixtures in laminar premixed burner-stabilized stagnation flames".

Three faculty members of the CCE were recognized as Thousand Young Talents.









Prof. Rémy Mével Prof. (2017)

Prof. Yu-Cheng Liu (2017)





#### **International Combustion Symposium Services**

 Prof. Xiaoqing You was appointed as a Colloquium Co-Chair for the 37th International Symposium on Combustion, colloquium on "Soot, Nanomaterials, and Large Molecules".
 Prof. Bin Yang was appointed as a Colloquium Co-Chair for the 37th International Symposium on Combustion, colloquium on "Gas-phase Reaction Kinetics".

#### Journal Editorial Services

- 1) Prof. Chao Sun is an Associate Editor for the International Journal of Multiphase Flow.
- 2) Prof. Zhuyin Ren is a member of the Editorial Board of Combustion Theory and Modelling.
- 3) Prof. Haitao Xu is a member of the Editorial Board of New Journal of Physics.
- 4) Prof. Suyuan Yu is a member of the Editorial Board of International Journal of Nuclear Energy Science and Technology.
- 5) Prof. Bin Yang is an Associate Editor of Combustion Science and Technology.

# **CCE Beacon Seminar Series**



#### Feb. 23, 2017

Mar. 1, 2017

Prof. **Rémy Mével**, CCE, Tsinghua University "Detonation Waves Structure and Dynamics"



# Prof. **Yu-Qing Lou**, Tsinghua University "Polar Magnetospheric Activities of Jupiter and Its Inner Radiation Belt"

Mar. 9, 2017

Mar. 23, 2017



Dr. **Tao Ren**, University of Californina at Merced "Radiative heat Transfer in Combustion"



Prof. **Wen Liu**, Beijing University of Chemical Technology "Surface Chemistry and Electrode

Design of Battery Electro-Catalysis"





#### April 6, 2017

Prof. **Mark Weislogel**, Portland State University highlighted "Strange Fluids Research in Space with Impacts to Space Exploration"

#### April 20, 2017



Prof. **Peng Zhang**, Hong Kong Polytechnic University "Theory of Circulation-controlled Fire Whirls"

#### May 11, 2017

May 25, 2017



Prof. **Zhensu She**, Peking University "Theory of Turbulent Boundary Layer and Design of Engineering Turbulence Model based on Symmetry Principle"

# R

Prof. Deanna A. Lacoste, KingAbdullah University"Influence of Non-Thermal PlasmaDischarges and Electric Fields on

Flame Dynamics"



Dr. **Riheng Zheng,** China Aerospace Science & Industry Corp "Current Situation and Challenges of Technology in Scramjet"

#### June 21, 2017

June 15, 2017



# Prof. **Peyman Givi**, University of Pittsburg

"Dynamic Partitioning and Quantum Speedup for Turbulent Combustion Simulation"

#### June 22, 2017



Prof. **Matthias Ihme,** from Stanford University visited the CCE under the sponsorship of the Bernard Lewis Visiting Lecturers Fellowship program of the Combustion Institute. He gave two lectures, respectively on: (i) Advances in Turbulent Combustion Modeling for Gas-phase and Multiphase Combustion, and (ii) Novel Combustion Concepts.

#### June 27, 2017



Prof. Xinyu Zhao, University of Connecticut

"Radiative Heat Transfer in Turbulent Multiphase Combustion: High-Fidelity and Reduced-Order Modeling"



#### Oct.20, 2017

June 29, 2017

Prof. **Shoutang Shang,** Aviation Industry Corporation of China

"Basic Research of Aero-Engine Combustion Technology Development and Requirements Analysis"



Prof. **André L.Boehman**, University of Michigan

"Impact of Oxygenated Fuels on Soot Nanostructure and Sooting Tendency"



Sept.7, 2017 Prof. **Damir Valiev,** CCE at Tsinghua Unvierstiy

"Premixed Flame Acceleration And Deflagration-to-Detonation Transition"



Prof. **Yu-Cheng Liu**, CCE at Tsinghua University

"Combustion Experiments under Microgravity Conditions"

#### Nov.30, 2017

Nov.9, 2017



## Sept.21, 2017

Prof. **Michel Louge**, Cornell University "Statistical Mechanics of Hysteretic Capillary Phenomena: Predictions of Contact Angle On Rough Surfaces and Liquid Retention in Unsaturated Porous Media"



Prof. **Chunxiao Xu**, Beijing University of Aeronautics and Astronautics BUAA Minimum-Flow-Unit Based Wall Turbulence Prediction and Preliminary Application

#### Dec.7, 2017



Prof. **Claus-Dieter Ohl**, University of Magdeburg "The Look and Touch of Nanobubbles"



#### Oct.19, 2017

Oct.12, 2017

Dr. **Paul Hellier**, University College London UCL "Optimized Biofuel Molecular Structures for

Ignition Quality and Low Emissions"



Prof. **Jinjun Wang**, Tsinghua University "An Investigation of Synthetic Jet Vortex Rings Impinging Onto A Solid Wall"

#### Dec.21, 2017



Prof. **Peixue Jiang,** Tsinghua University "Fluid Flow and Convective Heat Transfer of Supercritical Pressure Fluids under Multi-Factors Effects"

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