AFRL-SR-AR-TR-04-

0170

REPORT DOCUMENTATION PAGE

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
29-02-2004	Final Technical Report	01-11-2000 – 30-10-2003

4. TITLE AND SUBTITLE
(U) Physical and Chemical Processes in Flames

5a. CONTRACT NUMBER

5b. GRANT NUMBER
F49620-01-1-0029

5c. PROGRAM ELEMENT NUMBER
61102F

6. AUTHOR(S)
Chung K. Law

5d. PROJECT NUMBER
2308

5e. TASK NUMBER
BV

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Department of Mechanical and
Aerospace Engineering
Princeton University
Princeton, NJ 08544

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR/NA
4015 Wilson Boulevard
Room 713
Arlington VA 22203-1954

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited

20040423 048

13. SUPPLEMENTARY NOTES

14. ABSTRACT

The objective of the present program was to study the structure and response of laminar premixed and nonpremixed flames with emphases on effects of high pressure, flame/flow unsteadiness, and chemistry. The investigations were conducted through laser-based experimentation, computational simulation with detailed chemistry and transport descriptions, and advanced mathematical analysis. Specific phenomena studied during the reporting period include the intrinsic pulsating instabilities of premixed and diffusion flames and the effects of stretch and radiation heat loss on the onset of pulsation and the associated extinction and flammability limits. Laminar flame speed data were acquired for several fuel mixtures at atmospheric pressure and methane/air at elevated pressures. Directed relation graph theory and computational simulation were applied to develop automatic computational algorithms for the simplification of detailed mechanisms to skeletal mechanisms and of skeletal mechanisms to reduced mechanisms, respectively. These contributions are expected to be useful to the general interests of AFOSR in the fundamental and practical issues of flame dynamics and chemical kinetics, turbulent combustion, soot formation, radiation hear transfer, flame extinction, stabilization, flammability, and supersonic combustion.

15. SUBJECT TERMS
Pulsating instability; flammability limits; laminar flame speeds; mechanism reduction; skeletal mechanism; ethylene oxidation; directed relation graph; computational singular perturbation; high-pressure combustion.

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Julian M. Tishkoff
Unclassified	Unclassif ied	Unclassified	UL	16	19b. TELEPHONE NUMBER (include area code) (703) 696-8478

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39.18

Final Report

PHYSICAL AND CHEMICAL PROCESSES IN FLAMES

(Grant Number: F49620-01-1-0029)

Submitted By:

Chung K. Law
Department of Mechanical and Aerospace Engineering
Princeton University
Princeton, NJ 08544

Phone: 609-258-5178
Fax: 609-258-6233
E-Mail: cklaw@princeton.edu

For Consideration By:

Dr. Julian M. Tishkoff
Air Force Office of Scientific Research

SUMMARY/OVERVIEW

The objective of the present program was to study the structure and response of laminar premixed and nonpremixed flames with emphases on effects of high pressure, flame/flow unsteadiness, and chemistry. The investigations were conducted through laser-based experimentation, computational simulation with detailed chemistry and transport descriptions, and advanced mathematical analysis. Phenomena studied include the development of intrinsic flamefront pulsating instability, the influence of aerodynamic stretch and radiation heat loss on its development, and its relation to extinction, and studies related to the development of detailed and simplified chemical kinetic mechanisms.

Specifically, the results show that in the absence of stretch and heat loss, the onset of pulsating instability is described well by the Sivashinsky criterion of $Ze(Le-1)>11$, where Ze is the Zeldovich number and Le the Lewis number. The presence of pulsating instability was found to narrow the flammability limits. The onset of pulsating instability and the subsequent flame extinction occur over very narrow ranges of the fuel concentration such that, while its effect is substantial, its presence cannot be readily detected. Furthermore, it is shown that positive stretch tends to promote pulsating instability while negative stretch retards it, which is complete opposite to the trend for cellular instability, and that the presence of radiation heat loss further narrows the range for the onset of instability and hence the flammability limits.

Studies on combustion chemistry have been proceeding in two directions. In the first, experimentation was performed for 1,3-butadiene in flow reactors, and results were used to compile a kinetic mechanism for its pyrolysis and oxidation. Laminar flame speeds also were acquired for several fuel mixtures at atmospheric pressure and methane/air at high pressures. A mixing rule was developed, emphasizing the importance of the adiabatic flame temperature, and the adequacy of the widely used methane mechanism, GRI-Mech, was scrutinized. In the second effort, mathematical theory and computational algorithms were developed for the simplification of detailed mechanism to skeletal mechanism using directed relation graph theory and of the skeletal mechanism to reduced mechanism using computational singular perturbation. As an illustration, a reduced mechanism was derived subsequently for ethylene, demonstrating surprising preservation of comprehensiveness in the description of the chemical responses under extensive variations of the thermodynamic states and combustion configurations of the system.

These results are expected to be useful to the general interests of AFOSR in the fundamental and practical issues of flame dynamics and chemical kinetics, turbulent combustion, soot formation, radiative hear transfer, flame extinction, stabilization, flammability, and supersonic combustion.

ACCOMPLISHMENTS

The research program has two major focuses, namely the unsteady dynamics of flames and the chemical kinetics of flames. These two focuses cover a substantial arena in the current research activities in fundamental combustion. Good progress has been made in both endeavors during the reporting period. Highlights of the accomplishments can be found in the annual reports submitted to the program director, as well as the journal papers that have appeared in print. Thus only a very brief summary of these works are mentioned in the following.

Unsteady Flame Dynamics

Most practical combustion situations involve turbulent flames. Under most situations the chemical reactions take place in narrow regions, constituting the so-called laminar flamelets. These laminar flamelets are subjected to the fluctuating shearing action of the turbulent eddies and under severe conditions can be locally extinguished. Furthermore, because of the intrinsic disparity in the diffusivities of the heat and reactants, the flame front can exhibit intrinsic instability in the forms of cellularity and pulsation of the flame surface. The presence of such instabilities can modify the burning rate and possibly even affect the state of extinction. The studies on effects of forced oscillation were accomplished primarily during the previous funding period; consequently, emphasis was placed on the intrinsic pulsating instability for the current reporting period. The intention is eventually to couple forced and intrinsic instabilities to explore combustion control through resonance. The following is a synopsis of the results and the understanding gained therein.

Pulsating Instabilities in Premixed Flames [1, 2]

It has been well established that premixed flames would exhibit pulsating instability for Le>1 mixtures when the criterion Ze(Le-1)>11 is satisfied, where Ze is the Zeldovich number and Le the Lewis number. Since Le for gas mixtures is typically close to 1, while Ze is less than 10, it has been the prevalent belief that pulsating instability does not occur for gaseous flames. Rather, extensive interest has been placed on solid flames though the Self-Propagating High-Temperature Synthesis processes because Le>>1 for solids. We have, however, come to realize that because of the progressive dominance of chain-terminating reactions relative to the chain-branching reactions near the states of extinction and flammability, the effective activation energy, hence Zeldovich number, can assume substantially larger values, leading to the satisfaction of the above criterion with the potential occurrence of pulsating instability.

In this study the onset and characteristics of pulsating instability in unstretched, planar, lean heptane/air [1] and rich hydrogen/air [2] flames, for which the Le is greater than unity, were

investigated computationally. The occurrence of pulsating instability was identified, with the pulsation being monochromatic and then bi-chromatic as the burning becomes weaker with changing equivalence ratio. In the presence of radiative heat loss extinction sets in shortly. For the heptane/air flames, the transition from steady to pulsating propagation occurs over an extremely narrow range in the fuel concentration such that the pulsating extinction mode can be easily missed, leading to inappropriate interpretation of the limits of extinction based on steady-state extinction. For hydrogen/air flames, the sharpness of the chemical kinetics renders the transition between steady and pulsating propagation quite non-monotonic. For example, at elevated pressures such as 20 atmospheres, increasing the fuel concentration can lead to steady propagation, pulsating propagation, and steady propagation again as the controlling chemistry changes from that of $H\text{-}O_2$ branching to HO_2 branching.

In addition, it is seen that the pulsating flames are quasi-steady in nature in that the period of oscillation is larger than the characteristic flame time. As such, the unsteady flame cannot recover once the instantaneous flame temperature is reduced below the corresponding steady-state extinction temperature.

Pulsating Instabilities in Diffusion Flames [3, 4]

While extensive studies have been performed for flamefront instabilities in premixed flames, only recently have corresponding studies on diffusion flames been conducted. The reason was that diffusion flame sheets are inherently stable. However, recent analytical studies on the diffusion flame structure, allowing for finite-rate kinetics, have identified the possible onset of instability.

Recognizing the potential importance of such phenomena, we have conducted both computational and experimental studies with real fuel/oxidizer systems, aiming to scrutinize the validity of the analytical findings. The studies adopted the spherical flame as the configuration for analysis because it is not affected by aerodynamics. It was determined subsequently that extinction occurs in both the transport-induced limit of low mass flow rate and radiation-induced limit of high mass flow rate. Pulsating instability was observed, both experimentally and computationally, near both limits. The pulsating frequency varies from a few Hz for methane flames to tens of Hz for hydrogen flames. Results of this nature are expected to be useful in the sensing and control of flames.

Effects of Stretch and Heat Loss in Pulsating Instabilities [5, 6, 7, 8, 9]

Effects of stretch and curvature on the pulsating instability of premixed flames have been investigated for Le>1 mixtures via the negatively stretched inwardly propagating spherical flame and the positively stretched counterflow flame. Computational and asymptotic analysis results

show that pulsating instability is suppressed by the former and promoted by the latter. This behavior is completely opposite to that for cellular flames, for which positive stretch tends to suppress instability, while negative stretch promotes it. In particular, for a given rich hydrogen/air mixture whose one-dimensional, freely propagating flame is pulsatingly unstable, the inwardly propagating flame initially propagates at the laminar flame speed when the flame radius is large. Oscillation subsequently develops and is then amplified, damped, and eventually suppressed as the flame propagates inward and the magnitude of stretch increases. For the positively stretched rich hydrogen/air counterflow flame, oscillation is initiated at an equivalence ratio much smaller than the one-dimensional rich threshold. Furthermore, the critical strain rate leading to pulsation is smaller than the corresponding static extinction limit, implying that the flame extinguishes in the pulsating instead of the steadily propagating mode such that the flammable range is narrowed accordingly.

The computationally determined pulsation limits using realistic chemistry and transport also were found to agree well with the asymptotic results based on simplified chemistry and transport, provided that the global activation energies and Lewis numbers were extracted appropriately from the laminar flame responses.

While analytical and computational results show that pulsating instability occurs for $Ze(Le-1) = 11 >> 1$, microgravity experiments conducted elsewhere showed that pulsating instability also occurred for sub-unity Le systems. The flammability limits also were narrowed. A computational study allowing for radiation heat loss then demonstrated that this loss mechanism indeed could be the cause for the narrowing of the flammability limits. This study was followed by an asymptotic analysis for radiation-affected stretched flames. The experimental and computational results were captured.

Flame Propagation and Kinetics [10, 11, 12]

A major focus of this program is to acquire experimental data on flame propagation and then to use these data to validate and develop kinetic mechanisms. We have been engaged in studies involving the simpler fuels, including hydrogen, methane, and the C_2 hydrocarbons ethane, ethylene, and acetylene. Recently we also have performed experiments on the C_3 hydrocarbons propane, propene, and propyne. For the present period we have moved into the C_4 group of fuels. The first one we attempted was 1,3-butadiene [10], which is a crucial intermediate in the

oxidation of higher hydrocarbons. In this study we first performed flow reactor experiments for its pyrolysis and oxidation over the temperature range of 1035-1185 K. Using these data, as well as those from the literature, a kinetic mechanism for 1,3 butadiene oxidation was developed.

Considerable effort also has been expanded towards acquiring experimental data on the laminar flame speed, and using them to guide the development of kinetic mechanisms. Our first effort [11] involved the determination of atmospheric laminar flame speeds of mixtures of air with ethylene, *n*-butane, toluene, ethylene-*n*-butane, ethylene-toluene, and *n*-butane-toluene. Binary fuel blends with 1-to-1, 1-to-2, and 2-to-1 molar ratios were examined. Experimentally, the laminar flame speeds were determined using digital particle image velocimetry (DPIV). Since the use of DPIV enables the mapping of the two-dimensional flow field ahead of the flame, the reference speed based on the minimum axial velocity point as well as the imposed strain rate can be identified simultaneously. The latter now can be determined unambiguously by the radial velocity gradient at the minimum velocity point. By systematically varying the imposed strain rate, the corresponding laminar flame speed was obtained through nonlinear extrapolation to zero strain rate. Computationally, the laminar flame speeds were simulated for all single-component fuel/air and binary fuel blend/air mixtures with a detailed kinetic model. Comparison of experimental and computed flame speeds shows generally good agreement. A semi-empirical mixing rule was developed. The mixing rule, which requires only the knowledge of the flame speeds and flame temperatures of the individual fuel constituents, is shown to provide accurate estimates for the laminar flame speeds of binary fuel blends under the conditions tested.

In the second of the efforts [12], using a specially designed high- and constant-pressure combustion chamber, the propagation and morphology of spark-ignited expanding spherical methane flames were imaged using Schlieren cinematography and a high-speed digital camera. Stretch-free laminar flame speeds were determined subsequently for methane-air flames at pressures up to 20 atm. and methane-oxygen-helium flames at pressures up to 60 atmospheres. Computational simulation using GRI-Mech 3.0 showed satisfactory agreement with the experimental data up to 20 atm., and moderate deviation for pressures above 40 atm. Markstein lengths, global activation energies, and overall reaction orders also were determined as functions of pressure, with the latter two parameters exhibiting non-monotonic behavior caused by the changeover from H-O_2 to HO_2 chemistry similar to that of the explosion limits of homogeneous hydrogen-oxygen mixtures.

Theories and Algorithms for Kinetic Mechanism Reduction [13, 14, 15]

When the present research program was initiated a few years ago, the stated objective was the development of comprehensive detailed mechanisms covering hydrocarbons all the way from methane to the C_7-C_8 range. While this objective is still very much the main focus, an additional goal has been identified, namely the development of mathematical theories and computational algorithms for the automatic reduction of detailed mechanisms to simpler ones without loss of comprehensiveness. This undertaking was motivated by two considerations. First, detailed mechanisms are simply too large for integration into the computation of combustion flow fields. For example, the class of mechanisms developed by Westbrook and co-workers at the Lawrence Livermore laboratories, consisting of hundreds of species and thousands of reactions, cannot be used even for the calculation of the one-dimensional laminar flame structure and the associated flame speed. Other smaller mechanisms, such as GRI-Mech for methane oxidation, cannot be used for turbulent flame calculations. The second motivation was that the continuing updating of detailed mechanisms as new experimental and *ab initio* computational data become available. Obviously it is not reasonable to expect that a manual reduction needs to be performed whenever a new mechanism appears.

Our foray into mechanism reduction was initiated a few years ago by proposing an augmented reduced mechanism (ARM) for methane oxidation. This mechanism has since been used extensively by many turbulent flame and engine modelers, with satisfactory results. We now have extended this mechanism to include NOx formation [13].

We have made two major contributions in terms of theory and algorithm development. To understand the significance of these contributions, let us consider the general procedure adopted in mechanism reduction. We start with a detailed mechanism, which consists of many species and elementary reactions. The calculation time can be estimated roughly as being proportional to the square of the number of species. This detailed mechanism then is simplified to a so-called skeletal mechanism by eliminating unimportant species and reactions. This skeletal mechanism then is simplified further to a reduced mechanism by assuming quasi-steadiness for some species and partial equilibrium for some reaction. Thus, while the skeletal mechanism still consists of only elementary reactions, the reactions for the reduced mechanism are lumped.

The crucial criterion in mechanism reduction is to preserve the comprehensiveness of the chemical phenomena that the original mechanism is supposed to describe. The reaction mechanisms for hydrocarbon oxidation are intrinsically very complex, being highly coupled and nonlinear in terms of the concentrations, temperature, and pressure. Another well known example is the three explosion limits of hydrogen oxidation. For a given temperature, increasing the

system pressure from a low value can render a mixture from non-explosive, to explosive, to non-explosive again, and to explosive again. Furthermore, the mechanisms are expected to describe extensive classes of combustion phenomena: from atmospheric combustion in furnace and boilers to high-pressure combustion in i.c. engines; from low-temperature ignition to high-temperature burning; from lean to rich reactions as the mixture equivalence ratio varies due to design or imperfect mixing; and from the slow smoldering combustion to rapid explosions.

In our approach we first generated skeletal mechanisms from a detailed mechanism using directed relation graph with specified accuracy requirement [15] and subsequently generated reduced mechanisms from the skeletal mechanisms using computational singular perturbation (CSP) based on the assumption of quasi-steady-state species [14]. Both stages of generation are guided by the performance of a perfectly stirred reactor for high-temperature chemistry and auto-ignition delay for low- to moderately-high-temperature chemistry. The demonstration was performed for a detailed ethylene oxidation mechanism consisting of 70 species and 463 elementary reactions, resulting in a specific skeletal mechanism consisting of 33 species and 205 elementary reactions, and a specific reduced mechanism consisting of 20 species and 16 global reactions. Calculations for laminar flame speeds and nonpremixed counterflow ignition using either the skeletal mechanism or the reduced mechanism show very close agreement with those obtained by using the detailed mechanism over wide parametric ranges of pressure, temperature and equivalence ratio.

It is emphasized that Refs. 14 and 15 are significant contributions to the theories of mechanism reduction.

Review Activities [16, 17]

Two review articles were written on the two major activities of the present program. Reference 16 is on the dynamics of laminar flames. It updates a previous review article on the same subject presented as an invited paper at the 22nd International Combustion Symposium in 1988. That article has enjoyed extensive citation, by both the laminar and turbulent flame communities. The present update already has accumulated an impressive list of citations. The second article, on the development of detailed and reduced mechanisms, is of an advocacy nature, bringing attention to the importance of accurate and comprehensive reaction mechanisms in simulating combustion and propulsion phenomena to the aerospace community.

Writing review articles is a major, though essential, undertaking. The P.I. is pleased to have contributed to the literature in this manner.

JOURNAL PUBLICATIONS

Pulsating Instabilities in Premixed Flames

1. "Steady and pulsating propagation and extinction of rich hydrogen/air flames at elevated pressures," by E. W. Christiansen, C. J. Sung, and C. K. Law, *Combustion and Flame* **124**, 35-49 (2001).
2. "The role of pulsating instability and global Lewis number on the flammability limit of lean heptane/air flames," by E. W. Christiansen, C. K. Law, and C. J. Sung, *Proceedings of the Combustion Institute* **28**, 807-814 (2000).

Pulsating Instabilities in Diffusion Flames

3. "A computational study of oscillatory extinction of spherical diffusion flames," by E. W. Christiansen, S.D. Tse, and C.K. Law, *Combustion and Flame* **134**, 327-337 (2003).
4. "Oscillatory extinction of spherical diffusion flames," by S.W. Yoo, E.W. Christiansen, and C.K. Law, *Proceedings of the Combust. Inst*itute **29**, 29-36 (2002).

Stretch and Heat Loss Effects in Pulsating Instabilities

5. "On curvature-affected pulsating instability in inwardly-propagating spherical flames," by C. J. Sung, C. J. Sun, and C. K. Law, *Combustion Science and Technology Communications* **1**, 7-10 (2000).
6. "On stretch-affected pulsating instability in rich hydrogen/air flames: asymptotic analysis and computation," by C.J. Sung, A. Makino, and C.K. Law, *Combustion and Flame* **128**, 422-434 (2002).
7. "Pulsating instability and extinction of stretched premixed flames," by E.W. Christiansen and C.K. Law, *Proceedings of the Combustion Institute* **29**, 61-68 (2002).
8. "Radiation induced instability of stretched premixed flames," by Y. Ju, C. K. Law, K. Maruta, and T. Niioka, *Proceedings of the Combustion Institute* **28**, 1891-1900 (2000).
9. "Stability analysis of near-limit stretched premixed flames," by S. Minaev, R. Fursenko, Y. Ju, and C.K. Law, *Journal of Fluid Mechanics* **488**, 225-244 (2003).

Flame Propagation and Kinetics

10. "Detailed kinetic modeling of 1,3-butadiene oxidation at high temperatures," by A. Laskin, H. Wang, and C. K. Law, *International Journal of Chemical Kinetics* **32**, 589-614 (2000).
11. "Determination of laminar flame speeds of fuel blends using digital particle image velocimetry: ethylene, n-butane, and toluene mixtures," by T. Hirasawa, C.J. Sung, A. Joshi, H. Wang, and C.K. Law, *Proceedings of the Combustion Institute* **29**, 1427-1434 (2002).
12. "Outward propagation, burning velocities, and chemical effects of methane flames up to 60 atmospheres," by G. Rozenchan, D.L. Zhu, and C.K. Law, *Proceedings of the Combustion Institute* **29**, 1461-1470 (2002).

Theories and Algorithms for Kinetic Mechanism Reduction

13. "Augmented reduced mechanisms for NO emission in methane oxidation," by C.J. Sung, C.K. Law, and J.-Y. Chen, *Combustion and Flame* **125**, 906-919 (2001).
14. "Theory of complex CSP for chemistry reduction and analysis," by T. Lu, Y. Ju, and C. K. Law, *Combustion and Flame* **126**, 1445-1455 (2001).
15. "A directed relation graph method for mechanism reduction," by T.F. Lu and C.K. Law, submitted.

Review Articles

16. "Structure, aerodynamics, and geometry of premixed flamelets," by C.K. Law and C.J. Sung, *Progress in Energy and Combustion Science* **26**, 459-505 (2000).
17. "Development of comprehensive detailed and reduced reaction mechanisms for combustion modeling," by C.K. Law, C.J. Sung, H. Wang, and T.F. Lu, *AIAA Journal* **41**, 1629-1646 (2003).

PREPRINTS AND REPORTS

1. "Modeling of flame dynamics in complex flows," by C. K. Law, Proceedings of the Third International Symposium on Scale Modeling, Nagoya, Japan, Sept. 10-13, 2000.

2. "A computational study on oscillatory extinction of spherical diffusion flames," by E.W. Christiansen, S.D. Tse, and C.K. Law, AIAA Paper No. 2001-1084, 39th Aerospace Sciences Meeting, January 8-11, 2001, Reno, NV, January 8-11, 2001.

3. "Complex CSP for chemistry reduction and analysis," by Tianfeng Lu, Yiguang Ju and C.K. Law, AIAA Paper No. 2001-0943, 39th Aerospace Sciences Meeting, Reno, NV, January 8-11, 2001.

4. "A computational study on oscillatory extinction of spherical diffusion flames," by E.W. Christiansen, S.D. Tse, and C.K. Law, AIAA Paper No. 2001-1084, 39th Aerospace Sciences Meeting, Reno, NV, January 8-11, 2001.

5. "Determination of laminar flame speeds using digital particle image velocimetry," by T. Hirasawa, C.J. Sung, Z.W. Yang, H. Wang, and C.K. Law, Paper No. 138, 2nd Joint Meeting of the US Sections of the Combustion Institute, Oakland, CA, March 25-28, 2001.

6. "Effects of aerodynamic stretch and curvature on flame pulsation," by C.J. Sung, A. Makino, and C.K. Law, Paper No. 262, 2nd Joint Meeting of the US Sections of the Combustion Institute, Oakland, CA, March 25-28, 2001.

7. "On stretch-affected pulsating instability in rich hydrogen/air flames: asymptotic analysis and computation," by C.J. Sung, A. Makino, and C.K. Law, Paper No. 262, Second Joint Meeting of the US Section of the Combustion Institute, Oakland, CA, March 25-28, 2001.

8. "Development of comprehensive detailed and reduced reaction mechanisms for combustion modeling," by C.K. Law, C.J. Sung, H. Wang, and T.F. Lu, Paper No. 2002-0331, 40th Aerospace Sciences Meeting and Exhibit, January14-17, 2002, Reno, NV.

9. "A computational simulation of the dynamics of cell evolution in flame propagation," J. Yuan, Y. Ju, and C.K. Law, Third Joint Meeting of the US Sections of the Combustion Institute, Chicago, IL, March 17-19, 2003.

10. "Analysis of radiation induced instability of stretched premixed flames," by S. Minaev, Y. Ju, and C.K. Law, Third Joint Meeting of the US Sections of the Combustion Institute, Chicago, IL, March 17-19, 2003.

PRESENTATIONS

Keynote and Named Lectures

1. "Modeling of flame dynamics in complex flows," Third International Symposium on Scale Modeling, Nagoya, Japan, Sept. 10-13, 2000. **Conference Keynote Lecture**

2. "Frontiers of combustion: from microgravity to microengines," College of Engineering, the University of Florida, Gainesville, FL, Oct. 19, 2000. ** Benton Lecture**

3. "The role of chemical kinetics and laminar flames in the modeling of turbulent flames," APS Division of Fluid Dynamics Conference, Washington, D.C., Nov. 19-21, 2000. **Conference Keynote Lecture**

4. "Advances and needs in flame research," Second Joint US Sections Meeting of the Combustion Institute, Oakland, CA, March 26-28, 2001. **Conference Keynote Lecture**

5. "Frontiers of combustion: from microgravity to microengines," Tsinghua University, Beijing, China, April 23, 2001. **Inaugural Lecture as Guest Professor**

6. "The role of chemical kinetics and laminar flames in turbulent flame modeling," Technical Meeting of the Canadian Section of the Combustion Institute, Montreal, Canada, May13-16, 2001. **Conference Keynote Lecture**

7. "Hydrogen economy in the global carbon problem," Forum on New Challenges in Energy and Combustion, National Central University, Jungli, Taiwan, March 27, 2003. **Conference Keynote Lecture**

8. "Advances and needs in flame research," Thirteenth Technical Meeting of the Taiwan Section of the Combustion Institute, Taipei, Taiwan, March 29, 2003. **Conference Keynote Lecture**

9. "Ignition kinetics and flame dynamics in hydrogen combustion," Third Mediterranean Combustion Symposium, Marrakech, Morocco, June 9-13, 2003. **Conference Keynote Lecture**

10. "Combustion characteristics of energetic liquid propellants," National Aerospace Conference, National Cheng Kung University, Tainan, Taiwan, Dec. 19, 2003. **Conference Keynote Lecture**

Invited Departmental Seminars and Conference Session Talks

1. "Some aspects of the ignition-extinction S-Curves in combustion phenomena," Department of Theoretical and Applied Mechanics, University of Illinois at Urbana-Champaign, IL, Oct. 12, 2000.

2. "Aerodynamics and chemistry in flame propagation and modeling," Department of Mechanical Engineering, University of Pennsylvania, Philadelphia, PA, April 5, 2001.

3. "Aerodynamics of flames," Department of Engineering Mechanics, Tsinghua University, Beijing, China, April 24, 2001.

4. "The role of chemistry in flames," Department of Thermal Engineering, Tsinghua University, Beijing, China, April 25, 2001.

5. "Overview of NASA program on microgravity combustion," Space Studies Board, National Research Council, Washington, DC, October 23, 2001.

6. "Development of comprehensive detailed and reduced reaction mechanisms for combustion modeling," 40th Aerospace Sciences Meeting and Exhibit, Reno, NV, January 14-17, 2002.

7. "Aerodynamics and chemistry in flame propagation and modeling," Department of Mechanical Engineering, University of Calgary, Alberta, Canada, March 11. 2002.

8. "Combustion in high speed flows," JASON Summer Study – Hypersonics, La Jolla, CA, June 21, 2002.

9. "Droplet combustion of multicomponent and energetic fuels," Department of Mechanical Engineering, New Jersey Institute of Technology, Newark, N.J., Nov. 13, 2002.

10. "Chemical kinetics and flame dynamics in hydrogen combustion," Department of Mechanical Engineering, University of California, Riverside, CA, January 10, 2003.

11. "Fundamental processes in droplet combustion and collision," Department of Mechanical Engineering, City College of New York, New York, NY, Feb. 6, 2003.

12. "Combustion phenomena of interest to IC engines," Global Fuels Technology, BP Research, Naperville, IL, May 1, 2003.

13. "Hydrogen economy in the global carbon problem," Department of Mechanical Engineering, Hong Kong University of Science and Technology, Hong Kong, August 27, 2003.

14. "Some thoughts and action items in mechanism development for combustion applications," Workshop on the Simulation of the Combustion of Real Fuels, NIST, Gaithersburg, MD, Sept. 4-5, 2003.

15. "Properties of propane combustion," Strategic Planning Meeting, British Petroleum Corp., Chicago, IL, Nov. 20, 2003.

PERSONNEL

Principal Investigator

C.K. Law

Faculty Collaborators

J.K. Bechtold (New Jersey Institute of Technology)
J.Y. Chen (Berkeley)
A. Makino (Shizuoka University, Japan)
C.J. Sung (Case Western)
H. Wang (Delaware)
Y. Ju (Princeton)

Post-Doctoral Fellows and Research Staff

T. Hirasawa
H.Y. Sun
S.D. Tse
D.L. Zhu

Graduate Students

E.W. Christiansen (Ph. D. 2002)
G. Jomaas (M.S. student)
T. Lu (Ph.D candidate)
G. Rozenchan (M.S. 2002)
H.Y. Wang (Ph.D. candidate)

SIGNIFICANT INTERACTIONS

1. **Contact:** The Dow chemical Company; Albert Harvey; (225) 353-4035

   Results: Use of comprehensively validated reduced chemical kinetic mechanism allows realistic description of methane oxidation chemistry

   Applications: In-house code development and use.

2. **Contact:** United Technology Research Corp.; M.D. Colket; (860) 610-7481

   Results: Use of comprehensively validated reduced chemical kinetic mechanism allows realistic description of methane oxidation chemistry

   Applications: In-house code development and use

3. **Contact:** Fluent, Inc.; Graham Goldin; (800) 445-4454

   Results: Use of comprehensively validated reduced chemical kinetic mechanism allows realistic description of methane oxidation with NOx formation

   Applications: Commercially available code for engine and burner simulation