

Fall Technical Meeting of the Western States Section of the Combustion Institute 2005

(WSS/CI 2005 Fall Meeting)

**Stanford, California, USA
17 – 18 October 2005**

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at the address below.

Western States Section/Combustion Institute
P.O. Box 969 M S 9052
Livermore, California 94551-0969

Phone: 925-294-3840

Fax: 925-294-2276

<http://wssci.us/>

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2005 Fall Meeting

TECHNICAL PROGRAM

MONDAY, October 17, 2005

7:00 Registration and Continental Breakfast: Oak West Lounge, Tresidder Memorial Union, Stanford University

8:00 Welcome and opening remarks (Oak West Lounge)

Welcome Remarks, Professor **Reginald Mitchell**, Stanford University, Meeting Chair

Opening Remarks, Professor **James Plummer**, Dean, School of Engineering, Stanford University

8:15 05F-1 **INVITED TALK**, Oak West Lounge,

Advances in Diode Laser Sensors for Combustion and Propulsion, Professor

Ronald K. Hanson,

Stanford University,

Chair: Prof. C.T. Bowman, Stanford University

Morning Session 1A, Oak West Lounge,

Diagnostics and Modeling,

Chair: Prof. D. Kyritsis, University of Illinois at Urbana-Champaign

9:00 05F-2 A Comparison of Infrared Light Emitting Diodes (IR-LED)

versus IR Helium-Neon (HeNe) Lasers for Tomographic

Reconstruction of Mean and RMS Fuel Concentration in

Combustors, **J.W. Girard**, **G.E. Bogin**, **J.H. Mack**, **J.-Y.**

Chen, and **R.W. Dibble**, University of California, Berkeley

9:20 05F-3 Investigation of Two-Color Polarization Spectroscopy (TCPS)

and Two-Color Resonant Four-Wave Mixing (TCRFWM)

for Detection of Atomic Hydrogen, **W.D. Kulatilaka**

and **R.P. Lucht**, Purdue University, and **B.D. Patterson** and

T.B. Settersten, Sandia National Laboratories, Livermore,

California

9:40 05F-4 Initial Characterization of the Laser-Induced Breakdown

Spectroscopy Plasma for Diagnostics, **F. Ferioli**, **G.A.**

Lithgow, **E.S. Simpson**, and **S.G. Buckley**, University of

California, San Diego

10:00 Break

10:30 05F-5 Reaction Zone Structure in Lifted-Jet Partially-Premixed

Flames, **K.A. Watson**, University of the Pacific, **K.M. Lyons**,
North Carolina State University, and **C.D. Carter** and **J.M.**

Donbar, Air Force Research Laboratory

10:50 05F-6 A Correction to the PSR FORTRAN Code for the Accurate
Computation of the Inlet Composition, **N. Krishnamoorthy**

and **P.J. Smith**, University of Utah

11:10 05F-7 A New Technique for Apriori Evaluation of Combustion

Models, **J.C. Sutherland**, Sandia National Laboratories,
Livermore, California, **P.J. Smith**, University of Utah, and

J.H. Chen and **E. Hawkes**, Sandia National Laboratories,

Livermore, California (Paper 05F-8 withdrawn)

11:50 Lunch

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Morning Session 1B, Oak East Lounge,

Laminar Flames

Chair: Prof. J.-Y. Chen, University of California, Berkeley

9:00 05F-9 Ignition of the Butene Isomers: An Experimental and Kinetic
Study, **X.L. Zheng**, **H.Y. Sun**, and **C.K. Law**, Princeton

University

9:20 05F-10 Reacting Flow Computations with Reduced Chemical
Mechanisms, **H. Najm**, Sandia National Laboratories,
Livermore, California, **S. Iams**, University of Cambridge, **M.**

Valorani and **F. Creta**, University of Rome, and **D. Goussis**

9:40 05F-11 Pressure and Temperature Effects on the Flammability Limits
of CH₄/Air and C₃H₈/Air Flames, **A.T. Holley** and **F.N.**

Egolfopoulos, University of Southern California, and **C.K.**

Law, Princeton University

10:00 Break

10:30 05F-12 Comparison of Carbon Dioxide and Helium as Fire
Extinguishing Agents for Spacecraft, **Y. Son**, **G. Zouein**, and

P.D. Ronney, University of Southern California, and **S. Gokoglu**, NASA Glenn Research Center

10:50 05F-13 A Detailed Study of CO/H₂ Oxidation Kinetics in Synthesis-Gas/Air Premixed Flames, **D. Sheen**, **R. Kinslow**, **A.T. Holley**, **X. You**, **H. Wang**, and **F.N. Egolfopoulos**,

University of Southern California

11:10 05F-14 Numerical Simulations of Planar Unstrained Diffusion Flames, **S.R. Biles**, **M.S. Jakulewicz**, and **P. Papas**, Colorado School of Mines, and **D.G. Goodwin**, California

Institute of Technology

11:30 05F-15 Diffusion and Reaction Effects on iso-C₈H₁₈ Flame Ignition,

M.G. Andac and **F.N. Egolfopoulos**, University of Southern California

11:50 Lunch

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Morning Session 1C, Cypress South

Solid Fuel Burning, Flame Spread, and Detonations

Chair: **D. Rich**, University of California, Berkeley

9:00 05F-16 An Analysis of Upward Burning Utilizing Experimentally Measured Stand-off Distances, **A.S. Rangwala** and **S.G.**

Buckley, University of California, San Diego, and **J.L. Torero**, University of Edinburgh

Å

9:20 05F-17 The Effects of Wind on Crown Fire Initiation, **W.**

Tachajapong and **X. Zhou**, University of California, Riverside, **D. Weise**, Forest Fire Laboratory, Pacific Southwest Research Station, and **S. Mahalingam**, University

of California, Riverside

9:40 05F-18 Fuel Concentration Measurements During Flame Spread in Stratified Gas Mixtures, **M.J. Kulis** and **D.S. Perry**,

University of Akron, and **F.J. Miller** and **J.W. Easton**, National Center for Space Exploration Research

10:00 Break

10:30 05F-19 Flaming Ignition of Combustion Modified Polyurethane Foam, **O. Putzeys** and **A.C. Fernandez-Pello**, University of

California, Berkeley

10:50 05F-20 Coal Particle Ignition and Devolatilization During Oxygen-enhanced

and Oxygen/Carbon Dioxide Pulverized Coal
Combustion, **A. Molina** and **C.R. Shaddix**, Sandia National
Laboratories, Livermore, California

11:10 05F-21 Detailed and Reduced Chemical Reaction Mechanisms for
Detonation Simulation, **S. Browne**, **Z. Liang**, and **J.E.**
Shepherd, California Institute of Technology

11:30 05F-22 The Time-History of a DDT: Detonation Initiation by Thermal
Power Deposition on the Microsecond Time Scale, **D.R.**
Kassoy and **M. Nabity**, University of Colorado

11:50 Lunch

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1:10 05F-23 **INVITED TALK**, Oak West Lounge,
Some Innovative Applications of Combustion Science and Technology, Professor
Paul D. Ronney,
University of Southern California,
Chair: Prof. D. Dunn-Rankin, University of California, Irvine

Afternoon Session 1B, Oak West Lounge
**Practical Combustion Systems and Innovative Combustion
Concepts**

Chair: Prof. P.D. Ronney, University of Southern California

1:55 05F-24 Study of Rich Catalytic Combustion of Syngas as a First
stage in a Rich-Quick-Lean (RQL) Turbine System, **Y.F.**
Tham and **J.-Y. Chen**, University of California, Berkeley

2:15 05F-25 Experimental Investigation of Mesoscale Boundary Layer
Flows over Catalytic Surfaces, **S.A. Smyth**, **K. Bijjula**, and
D.C. Kyritsis, University of Illinois at Urbana-Champaign

2:35 05F-26 Hydrogen Combustion in Mesoscale Burner Arrays for Gas
Turbine Applications, **E.A. Gonzales**, **K. Walters**, **A.**
Bardosova, **S. Lee**, and **C.T. Bowman**, Stanford University

2:55 05F-27 Effects of Hydrogen on Centimeter-Scale Four-Stroke
Engine, **J. Pompa**, **S. Karnani**, **A. Mulrone**, **A. Leal, Jr.**,
and **D. Dunn-Rankin**, University of California, Irvine

3:15 Break

3:45 05F-28 Effect of Wall Thermal Conductivity and Thickness on the

Performance of Heat-Recirculating Reactors, **J. Ahn** and **P.D. Ronney**, University of Southern California

4:05 05F-29 Electric Field Effect on Oxygen-Enriched CH₄/O₂/N₂ Premixed Flames **K.Y. Lee**, **S.S. Shin**, and **E. Vega**, Andong National University

4:25 05F-30 Voltage-Current Characteristics of Small Diffusion Flames under the Combined Influence of Ion-Driven Winds and Natural Convection **M.J. Papac**, **P. Chueh**, and **D. Dunn-Rankin**, University of California, Irvine, and **F.J. Weinberg**, Imperial College

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Afternoon Session 2B, Oak East Lounge

Turbulent Combustion

Chair: Prof. H. Pitsch, Stanford University

1:55 05F-31 Joint Scalar Probability Density Function Simulation of a Single Burner Test Furnace with Ultra-Low NO_x Gas Burner, **Q. Tang**, **M. Denison**, **M. Bockelie**, and **M. Cremer**, Reaction Engineering International, and **D. Brown**, Stone & Webster, Inc

2:15 05F-33 LES of Sandia Flame D with Eulerian PDF and Finite-Rate Chemistry, **F. Bisetti** and **J.-Y. Chen**, University of California, Berkeley (Paper 05F-32 withdrawn)

2:35 05F-34 A New Solver for Large-Eddy Simulations of Turbulent Premixed Combustion in Complex Geometries, **V. Moureau** and **H. Pitsch**, Stanford University

2:55 05F-35 Large Eddy Simulation of a Turbulent Jet Diffusion Flame Stabilized on a Bluff-Body: Characteristics of the Mixing Field and NO Formation, **S.H. Kim** and **H. Pitsch**, Stanford University

3:15 Break

3:45 05F-36 Numerical Simulations of Turbulent Bluff-body Flames using Multi-environment Presumed PDF Method with Realistic Chemistry, **Q. Tang**, **W. Zhao**, **M. Bockelie**, and **M. Cremer**, Reaction Engineering International, and **R. Fox**, Iowa State University

4:05 05F-37 Joint Probability Density Function Model Validation by Experimental Flame Data, **D. Yeates** and **P. Smith**, University of Utah

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Afternoon Session 2C, Cypress South

Chemical Kinetics and Mechanism Development

Chair: Dr. D. Golden, Stanford University

1:55 05F-38 Unimolecular Reactions in Combustion Databases, **W.**

Tsang, National Institute of Standards and Technology

2:15 05F-39 Modeling Benzene and Naphthalene Formation in a Premixed Propylene Flame, **H.R. Zhang, E.G. Eddings**, and

A.F. Sarofim, University of Utah

2:35 05F-40 High Temperature Measurements of the Reactions

$\text{CH}_2\text{O} + \text{M} = \text{Products}$ and $\text{CH}_2\text{O} + \text{O}_2 = \text{Products}$, **V. Vasudevan**,

R.K. Hanson, C.T. Bowman, and **D.M. Golden**, Stanford

University

2:55 05F-41 Flow Reactor Pyrolysis of Diethyl Sulfide, **X. Zheng, E.M.**

Fisher, and **F.C. Gouldin**, Cornell University, and **L. Zhu**

and **J.W. Bozzelli**, New Jersey Institute of Technology

3:15 Break

3:45 05F-42 Thermochemical Properties for N-Butyl and N-Pentyl

Hydroperoxides, the Alkyl and Peroxy Radicals, Transition

States and Kinetics for Intramolecular Hydrogen Shift

Reactions to the Peroxy Radicals, **L. Zhu, L.M. Kardos, C.J.**

Pope, and **J.W. Bozzelli**, New Jersey Institute of Technology

4:05 05F-43 Reporting of Experimental Data for Development and

Validation of Chemical Kinetic Models, **Z.M. Djurisic** and **M.**

Frenklach, University of California, Berkeley, and **T. Allison**,

National Institute of Standards and Technology

4:25 05F-44 Development of Isooctane Skeletal Mechanisms for Fast and

Accurate Predictions of SOC and Emissions of HCCI

Engines Based on LLNL Detailed Mechanism, **Y.-H. Chen**

and **J.-Y. Chen**, University of California, Berkeley

5:00-6:30 Reception (Student Awards) and Laboratories Visit

Location: MERL (new Mechanical Engineering Research Laboratories)

2005 Fall Meeting

TECHNICAL PROGRAM

TUESDAY, October 18, 2005

7:30 Continental Breakfast: Oak West Lounge, Tresidder Memorial Union, Stanford University

8:30 05F-45 **INVITED TALK**, Oak West Lounge,
Physically-Based Modeling of Solid Oxide Fuel Cells: From Elementary Reaction Mechanisms to Engineering Performance Prediction, Professor David Goodwin, California Institute of Technology,
Chair: Prof. H. Wang, University of Southern California

Morning Session 3A, Oak West Lounge

Nanoparticles and Soot

Chair: Dr. A. Molina, Sandia National Laboratories, Livermore, California

9:15 05F-46 Ultrafine Anatase TiO₂ Nanoparticles Synthesized Using an Atmospheric Premixed Stagnation Flame, **B. Zhao, K. Uchikawa**, and **H. Wang**, University of Southern California, and **J.R. McCormick** and **J.G. Chen**, University of Delaware

9:35 05F-47 A Unipolar Corona Ionizer for Charging Nanometer-size Particles, **K. Hinckley**, University of California, Berkeley, **D. Lucas**, Lawrence Berkeley National Laboratory, **L. Sgro**, Università degli Studi di Napoli, **C. Koshland**, University of California, Berkeley, **G. Lanzuolo**, Università di Napoli, and **R. Sawyer**, University of California, Berkeley

9:55 05F-48 Soot Formation in Diesel Combustion under High-EGR Conditions, **C.A. Idicheria** and **L.M. Pickett**, Sandia National Laboratories, Livermore, California

10:15 Break

10:45 05F-49 Bimodal Particle Size Distributions and Morphology of Soot in a Laminar Premixed Ethylene Flame, **K. Uchikawa, B. Zhao**, and **H. Wang**, University of Southern California

11:05 05F-50 Modeling Soot Formation in Counterflow Diffusion Flames by Sectional Method, **Z. Yang, D.O. Lignell**, and **N. Krishnamoorthy**, University of Utah, and **H.K. Moffat, S.R. Tieszen**, and **J.C. Hewson**, Sandia National Laboratories, Livermore, California

11:25 05F-51 Laser Extinction in Laminar Inverse Diffusion Flames, **K.T. Macko, M.A. Mikofski, A.A. Bar-Ilan**, and **A.C. Fernandez-Pello**, University of California, Berkeley, and **L.G. Blevins**, Sandia National Laboratories, Livermore, California

11:45 Lunch

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Morning Session 3B, Oak East Lounge

Droplets, and Practical and Surrogate Fuels

Chair: P. Pepiot, Stanford University

9:15 05F-52 Liquid Fuel Burning with Non-Unitary Lewis Number, **W.A.**

Sirignano, University of California, Irvine

9:35 05F-53 Effects Of Supporting Rods On Methanol Droplet Heating and Vaporization with Surface Tension Effects, **D. Shringi,**

H.A. Dwyer, and **B.D. Shaw**, University Of California, Davis

9:55 05F-54 Reduced Gravity Combustion of Propanol Droplets with Various Inert Gases, **J. Wei** and **B.D. Shaw**, University of

California, Davis

10:15 Break

10:45 05F-55 The Autoignition of JP-8, Jet-A, and Selected Reference Components in a Single Cylinder Engine, **R. Johnson, R.**

Natelson, M. Kurman, N.P. Cernansky, and **D. Miller**,

Drexel University

11:05 05F-56 Ignition and Extinction of Non-Premixed Flames of Single-Component Liquid Hydrocarbons, Jet Fuels and their Surrogates, **A.T. Holley, Y. Dong, M.G. Andac**, and **F.N.**

Egolfopoulos, University of Southern California, and **J.T.**

Edwards, Air Force Research Laboratory

11:25 05F-57 Soot Volume Fraction from Extinction in JP8 and Heptane Pool Fires, **T. Henriksen**, University of Utah, **G. Nathan** and

Z. Alwahabi, University of Adelaide, and **J. Spinti, E.**

Eddings, and **P. Smith**, University of Utah

11:45 Lunch

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Morning Session 3C, Cypress South

Kinetics and Pollutants

Chair: Dr. Z.M. Djurisic, University of California, Berkeley

9:15 05F-58 Direct Determination of the Dominant CH(A) Formation Reaction, **J.M. Hall** and **E.L. Petersen**, University of Central Florida

9:35 05F-59 Thermal Decomposition of Toluene: Overall Rate and Branching Ratio, **M.A. Oehlschlaeger**, **D.F. Davidson**, and **R.K. Hanson**, Stanford University

9:55 05F-60 A Shock-Tube Study of The Ignition and Oxidation Characteristics of CO/H₂ Fuel Blends in Air, **D. Kalitan** and **E. Petersen**, University of Central Florida, and **M. Crofton**, The Aerospace Corporation

10:15 Break

10:45 05F-61 Methyl Concentration Time Histories during iso-Octane and n-Heptane Oxidation and Pyrolysis, **D.F. Davidson**, **M.A. Oehlschlaeger**, and **R.K. Hanson**, Stanford University

11:05 05F-62 Graphene Layer Growth: Collision of Migrating 5-member Rings, **R. Whitesides**, **A.C. Kollias**, **D. Domin**, **W.A. Lester, Jr.**, and **M. Frenklach**, University of California, Berkeley

11:25 05F-67 A Modeling and Experimental Investigation of Methylcyclohexane in a Rapid Compression Machine, **W.J. Pitz**, Lawrence Livermore National Laboratory, Livermore, California, **C.V. Naik**, Colorado School of Mines, **T.N. Mhaoldúin**, **H.J. Curran**, **J.P. Orme**, and **J.M. Simmie**, National University of Ireland, Galway, and **C.K. Westbrook**, Lawrence Livermore National Laboratory, Livermore California (Paper 05F-63 Withdrawn)

11:45 Lunch

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1:00 05F-64 **INVITED TALK**, Oak West Lounge,
A Low-Greenhouse-Gas Energy Future: Technical Challenges to the Scientific Community, **Professor Christopher F. Edwards**,
Stanford University,
Chair: Prof. Reginald Mitchell, Stanford University

Afternoon Session 4A, Oak West Lounge
Turbulent Combustion and Kinetics
Chair: Dr. V. Moureau, Stanford University

1:45 05F-65 Resolution/Noise Effects for Thermal Dissipation

Measurements in a Turbulent Non-Premixed Jet Flame, **G. Wang** and **R.S. Barlow**, Sandia National Laboratories, Livermore, California, and **N.T. Clemens**, University of Texas at Austin

2:05 05F-66 CO and NO_x Emissions of Strongly-Pulsed Turbulent Jet Diffusion Flames, **M. Fregeau**, **P.-Y. Tsai**, and **C. Hermanson**, University of Washington

2:25 Break

2:55 05F-68 Flamelet-Based Modeling of H₂/Air Auto-Ignition with Thermal Inhomogeneities, **D.J. Cook**, Stanford University, **J.H. Chen**, **E.R. Hawkes**, and **R. Sankaran**, Sandia National Laboratories, Livermore, California, and **H. Pitsch**, Stanford University

3:15 05F-69 Large Eddy Simulation of Turbulent Reacting Mixing Layers, **P. Prasad**, **X. Zhou**, and **S. Mahalingam**, University of California, Riverside

2005 Fall Meeting

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Afternoon Session 4B, Oak East Lounge

General Topics and Practical and Surrogate Fuels

Chair: Dr. M. Oehlschlaeger, Stanford University

1:45 05F-70 Supercritical Combustion: A Fresh Look at an Old Concept, **J.A. Cole**, Quantum Energy Technologies Corp.

2:05 05F-71 Field Performance of a Nephelometer in Rural Kitchens: Effects of High Humidity Excursions and Correlations to Gravimetric Analyses, **S.L. Fischer** and **C.P. Koshland**, University of California, Berkeley

2:25 Break

2:55 05F-72 Evaluating the HCCI Characteristics of Hexane and Pentane in a Rapid Compression Expansion Machine, **S. Goldsborough**, Marquette University, and **P. Van Blarigan**, Sandia National Laboratories, Livermore, California

3:15 05F-73 Relationship Between Ignition Processes and the Lift-Off Length of Diesel Fuel Jets, **L.M. Pickett**, **D.L. Siebers**, and **C.A. Idicheria**, Sandia National Laboratories, Livermore, California

3:35 05F-74 Ignition and Extinction of Mixtures of Pure Liquid Hydrocarbons, Samples of Gasoline, and Gasoline Surrogates with Air, **A.T. Holley**, **Y. Dong**

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Afternoon Session 4C, Cypress South

Particulate Emissions, Pollutants, and Flame Stabilization

Chair: Dr. M.G. Andac, University of Southern California

1:45 05F-75 The Influence of Biodiesel on the Kinetics of Exhaust Particle Oxidation and Emissions, **H. Jung**, University of California, Davis, **D.B. Kittelson**, University of Minnesota, and **M.R.**

Zachariah, University of Maryland  G F

2:05 05F-76 Particle and Gas Emissions from a Simulated Household Fire Pit, **L. Tian**, University of California, Berkeley, **D. Lucas**, Lawrence Berkeley National Laboratory, **S.L. Fischer**, University of California, Berkeley, **S.-C. Lee**, Hong Kong Polytechnic University, and **C.P. Koshland**, University of California, Berkeley  G E

2:25 Break

2:55 05F-77 A Numerical and Experimental Investigation into the Anomalous Slight NO_x Increase When Burning BioDiesel, **G.**

Ban-Weiss, R. Gupta, J.-Y. Chen, and R.W. Dibble, University of California, Berkeley  H E J

3:15 05F-78 Investigation of Flame Stabilization and NO Production in a Plasma Assisted Methane/air Premixed Flame, **W. Kim, H.**

Do, G. Mungal, and M. Cappelli, Stanford University  H I