

**MULTI AGENCY COORDINATION COMMITTEE FOR COMBUSTION RESEARCH
(MACCCR) -- 5th Annual FUELS RESEARCH REVIEW**

**Combustion Research Facility (CRF), Sandia National Laboratory
September 17-20, 2012**

Monday, September 17

0800 – 0815 Welcome and Opening Remarks: Dawn Manley, Sandia/CRF and Wade Sisk, DOE/BES

Keynote Presentation, Chair: Ralph Anthenien

0815 – 0900 Fuel Effects on Combustion, Tim Edwards, AFRL/RZ

Supercritical Fuel and Soot, Chair: Ralph Anthenien

0900 - 0930 Supercritical Fuel Pyrolysis, Judy Wornat, Louisiana State University

0930 - 1000 Mechanism of Soot Formation: Oxidation, Michael Frenklach, UC Berkeley

1000 - 1030 BREAK

Fuel and Combustion Chemistry, Chair: Ralph Anthenien

1030 - 1100 Experimental Study of the Oxidation, Ignition, and Soot Formation Characteristics of Jet Fuel, Matthew Oehlschlaeger, Rensselaer Polytechnic Institute

1100 -1130 Shock Tube/Laser Absorption Studies of Jet Fuels at Low Temperatures (600-1200K), Ronald Hanson, Stanford University

1130 - 1200 Characterization of RP-1 Kinetics during Pyrolysis and Oxidation, David Davidson and Ronald Hanson, Stanford University

1200 - 1300 Lunch

Combustion Chemistry, Chair: Chiping Li

1300 - 1330 High Temperature Reactions of Fuels and Fuel Radicals, Wing Tsang, National Institute of Standards and Technology

1330 - 1400 Intermediate Temperature Autoignition Chemistry of Fuels, John Dec, Sandia/CRF

1400 - 1430 Autoignition chemistry of biofuels, Craig Taatjes, Sandia/CRF

1430 - 1500 Detailed and Simplified Chemical Kinetics of Aviation Fuels and Surrogates
Peter Lindstedt, Imperial College of Science, Technology, and Medicine

1500 - 1530 Break

Combustion Cyber Infrastructure, Chair: Wade Sisk

1530 – 1600 PrIme Next Frontier: Large, Multi-dimensional Data Sets, Michael Frenklach, UC Berkeley

1600 – 1630 NIST Presentation, Pam Chu/Jeffrey Manion, NIST

1630 – 1700 MACCCR Workshop Presentation, Phil Westmoreland, NCSU

1700 – 1800 Free Format Discussion on Combustion Cyber Infrastructure

Tuesday, September 18

0800– 0815 Announcements

Keynote Presentation, Chair: Dawn Manley

0815 - 0900 Fuel Research at UTRC, Meredith Colket, UTRC

Turbulent Flame and Reactive Flow Simulation, Chair: Dawn Manley

0900 - 0930 Multi-scalar Experiments on Turbulence-Chemistry Interaction, Robert Barlow, Sandia/CRF

0930 - 1000 DNS for Turbulent Flame, Jacqueline Chen, Sandia/CRF

1000 - 1030 Break

Turbulent Flame and Reactive Flow Simulation, Chair: Dawn Manley

1030 – 1100 LES for Multiphase Turbulent Reactive Flows, Joe Oefelein Sandia/CRF

1100 – 1130 Engine Combustion Network: International Spray Combustion Research Collaboration for Engine Fuel Sprays, Lyle Pickett, Sandia/CRF

1130 - 1300 Lunch

Combustion Kinetics and Flame Modeling, Chair: Wade Sisk

1300 – 1530 DOE/BES CEFRC Highlights
CEFRC Overview, Chung King Law, Princeton University
Butanol Mechanism Thrust, William Green, MIT
Uncertainty in A Priori Kinetics Predictions, Stephen Klippenstein, Argonne
Flame Chemistry and Biodiesel Kinetics, Yiguang Ju, Princeton University
High-Fidelity Simulations of Turbulent Combustion, Jacqueline Chen

1530 - 1545 Break

1545 - 1800 Sandia/CRF Visit

Wednesday, September 19

0800– 0815 Announcements

Turbulence and Chemistry Interaction, Chair: Chiping Li

0815 - 1200 AFOSR Energy IPT
Fokion Egolfopoulos, University of Southern California
Hai Wang, University of Southern California
Chung King Law, Princeton University
Ronald Hanson, Stanford University
Tom Bowman, Stanford University
Nicholas Cernansky, Drexel University
David Miller, Drexel University

1200 - 1300 Lunch

Fuels and Surrogates, Chair: Tim Edwards

1300-1330 Fuel Research Review, Charlie Westbrook, LLNL

1330-1400 Fuel Surrogate Mechanisms, William Pitz, LLNL

1400-1430 Autoignition Chemistry of Surrogate Fuel Components in an Engine Environment, David Miller, Drexel University

1430-1500 Development of Surrogate Model Fuel for F-76, YoungChul Ra/Rolf Reitz, UW-Madison

1500-1530 Methods for formulating diesel surrogates, Chuck Mueller, Sandia/CRF

Break 1530 – 1550

Future Direction in Surrogate Fuel Research – Panel Discussion, Moderator: Chiping Li, Panel Members: Ralph Anthenien, Tim Edwards, Hai Wang, Chris Shaddix, Meredith Colket and Fred Dryer

1550-1555 Opening Remarks, Chiping

1555-1630 Generation of Comprehensive Surrogate Kinetic Models and Validation Data Bases for Simulating Large Molecular Weight Hydrocarbon Fuels (Concluding Summary for this 2007 MURI), Fred Dryer, Princeton University

1630-1635 Meredith Colket, UTRC

1635-1640 Tim Edwards, AFRL

1640-1645 Hai Wang, USC

1645-1650 Chris Shaddix, Sandia/CRF

1650-1830 Discussion

Thursday, September 20

0800 - 0815 Announcements

Computational Method for Combustion Problems, Chair, Jacqueline Chen

0815 – 0900 UQ and Chemical Model Reduction, Habib Najm, Sandia/CRF

0900 – 0930 Chemical Kinetic and Transport Model Uncertainty Analyses and Mechanism Reduction for Propulsion Systems: From SCRAM Jets to Gas-Turbine Propulsion Systems, Harsha Chelliah, UVA

0930 – 1015 Numerical Simulations of Chemically Reacting Flow and Experiments on Jet Fuel and Its Surrogates at Pressures, Mitchell Smooke, Yale University

1015 - 1045 Modeling of Conserved Scalars under Supercritical Pressure Condition, Josette Bellan, NASA/JPL

Lunch 1045 – 1145

*Workshop – Future Directions and Opportunities of Combustion Chemistry Research)
Chair, Chiping Li*

1145 –1200 Agency's Perspectives: Ralph Anthenien, Tom Settersten, and Chiping Li

1200-1230 New Approaches to Reacting Flow Modeling for Endothermic Fuel Cracking and Combustion in High-Speed Combustion, Hai Wang, USC

1230-1300 Multi-Scale Interaction of Vibrational Energy Transfer and Turbulent Combustion in Supersonic Flows, Phil Varghese, UT Austin

1300-1330 Supercritical Catalytic Cracking of Hydrocarbon Feeds – Insight into Selectivity and Stability Utilizing a Combined Kinetic and Operando non-Linear Spectroscopy Approach, Rob Rioux, Penn State

1300-1400 Characterization of Radical and Stable Species from Pyrolytic and Catalytic Endothermic Fuel Decomposition, Harsha Chelliah, UVA

1400-1430 Stationary Mixed Metal-Oxide Acid Catalysts for Endothermic Fuel Decomposition and Enhanced Ignition/Flame Holding Characteristics, Tony Dean, CSM

1430 –1600 Discussion on Ideas for Future Combustion Chemistry Research

1600 Adjourn