

2016 10th MACCR Annual Fuel and Combustion Research Review

Drs. Chiping Li and Wade Sisk | October 17-20, 2016 | ANL, IL

Argonne National Laboratory
Building 200 (Chemistry) Auditorium
Chicago, Illinois

Agenda Day 1 | Monday, October 17, 2016

Time	Title	Speaker
0900 - 0910	Opening and Welcome Remarks	DOE Argonne National Laboratory Leadership
0910 - 0915	Additional Remarks	Stephen Pratt/DOE-ANL, Ralph Anthenien/ARO, Song-Chang Kong/NSF and Chiping Li/AFOSR

Multi-Phase Combustion and Multi-Physics Modeling: Chair: Jeff Moder

0915 - 0945	Heavy-Alkane and Cyclohexane Reduced Oxidation Kinetics	Josette Bellan/JPL
0945 - 1015	Chemical Kinetics: The Evolving Roles of Theory, Experiment, and Modeling	Steve Klippenstein/ANL
1015 - 1045	Enabling Detailed Kinetics in the Simulation of Complex Reactive Flows	Perrine Pepiot/Cornell
1045 - 1115	Two-Phase CFD Simulation for Jet Engine Combustor Flows: Spray-Model Assumptions/Details and Comparison to Experiments	Matthias Ihme/Stanford
1115 - 1145	Multicomponent Microscale Droplet Impact Behavior with Heated Surfaces	James Michael/Iowa State
1145 - 1330	LUNCH	

Aviation Fuel and Combustion: Chair: Chiping Li

1330 - 1415	Summary of NASA NRA on Aviation Fuels and Combustion	Jeff Moder/NASA
1415 - 1445	Jet Fuel Flame Speed and Flammability Measurements	Fokion Egolfopoulos/USC
1445 - 1530	Perspective on Jet Fuel Physical Properties and Progress in NJFCP	Tim Edwards/AFRL
1530 - 1600	Jet Fuel Lean Blow-Out Experiments	Edwin Corporan and Scott Stouffer/AFRL
1600 - 1630	BREAK	

Special Invited Presentation on Novel Jet Engine Combustor Development: Chair: Chiping Li

1630 - 1715	History and Recent Progress in Trapped Vortex Combustor	Mel Roquemore/AFRL
Combustion Diagnostics: Chair: Chiping Li		
1715 - 1745	Cavity Enhanced Magneto-Optic Rotation (CEMOR)	Nike Cernansky/Drexel
1745 - 1815	4D Combustion Diagnostics	Lin Ma/Virginia Tech
MEETING ADJOURNED FOR THE DAY		

Agenda Day 2 Monday, October 18, 2016		
Time	Title	Speaker
0755 - 0800	Daily Announcements	Stephen Pratt/DOE-ANL, Ralph Anthenien/ARO, Song-Charng Kong/NSF and Chiping Li/AFOSR
High-Pressure, Multi-Phase and Super-Critical Fuel and Combustion: Chair: Ralph Anthenien		
0800 - 0845	Overview of High-Pressure Combustion Experimental Facility at ARL	Mike Kweon/ARL
0845 - 0915	Molecular Dynamics Simulation of Transcritical Fuel Properties	Li Qiao/Purdue
0915 - 0945	Molecular Modeling Interface for Predicting Properties of Fuels over a Broad Range of Conditions	Judith Harrison/USNA
0945 - 1000	BREAK	
1000 - 1030	High Pressure Ring Contraction of Cyclic Hydrocarbons	Ken Brezinsky/UIC
1030 - 1100	Hi-Pressure Kinetics via High Repetition Rate Diaphragmless Shock Tube	Rob Tranter/ANL
1100 - 1130	Direct Measurements of Critical Combustion Intermediates at Elevated Pressures	Leonid Sheps/SNL-CRF
1130 - 1300	LUNCH	
Special Topics in Combustion Chemistry: Chair: David Urban		
1300 - 1330	Prompt Dissociations of Small Combustion Radicals	Raghu Sivaramakrishnan/ANL
1330 - 1400	Effects of Explosive Ozonolysis Reactions on Jet	Wenting Sun/GATech

	Flame Stabilization	
1400 - 1415	Energy Kinetic Package (EKP, a Cantera Based Package for Combustion, Battery, Fuel Cell and Energy Related Catalytic Reactions) – on special invitation	Robert Kee/CSM
1415 - 1500	Combined Molecular Beams and Computational Study on the Decomposition of JP-8 and JP-10 - From Surrogates to Real Fuel	Ralp Kaiser/U Hawaii and Alexander Mebel/FIU
1500 - 1530	BREAK	
NSF/DOE Combustion Partnership on IC Engines: Chair: David Urban		
1530 - 1615	Highlights of NSF/DOE Partnership on Advanced Combustion Engines Initiative (2013 - 2016) and Future Opportunities	Song-Charng Kong/NSF
Microgravity Combustion: Chair: Song-Charng Kong		
1615 - 1700	Overview and Recent Progresses of NASA Microgravity Combustion Program	David Urban/NASA
Cool Flames: Chair: Chair: David Urban		
1700 - 1730	Some Recent Developments in Low-Temperature Flames	C.K. Law/Princeton
1730 - 1800	Cool Flames and In Situ Measurements of OH and HO	Yiguang Ju/Princeton
	MEETING ADJOURNED FOR THE DAY	

Agenda Day 3 Monday, October 19, 2016		
Time	Title	Speaker
0755 - 0800	Daily Announcements	Stephen Pratt/DOE-ANL, Ralph Anthenien/ARO, Song-Charng Kong/NSF and Chiping Li/AFOSR
Ab Initio, Pathway Centric Combustion Chemistry Approach Chair: Stephen Pratt		
0800 - 0900	Overview of MURI: New Theoretical and Experimental Methods for Predicting Fundamental Mechanisms of Complex Chemical Processes	Don Thompson/U Mo Columbia
0900 - 0930	Uncovering Complex Reaction Networks from First Principles	Todd Martinez/Stanford

0930 - 0945	BREAK	
0945 - 1115	Reaction Networks and Mechanisms: Discovery and Application in Combustion	Hai Wang/Sanford, Anna Krylov, James Pfaendtner/UW, and David Glowacki/U Bristol
1115 - 1145	Reaction Network Reconstruction for Modeling of Dynamic Pathways	Angela Violi/Michigan
1145 - 1330	LUNCH	
Low Temperature Combustion Chemistry and Its Strong Molecular Dependency: Chair: Ralph Anthenien		
1430 - 1500	A New Approach to the Combustion Chemistry of Low Cetane Number Jet Fuels	Ken Brezinsky/UIC
1500 - 1530	High pressure LTC Kinetics via Rapid Compression Machine	Margaret Wooldridge/Michigan
1530 - 1600	BREAK	
1600 - 1630	Low Temperature Combustion Experiments for Real HC Fuels	Matt Oehlschlaeger/RPI and Tonghun Lee/UIUC
1630 - 1700	High-Pressure, Low Temperature Jet Fuel Combustion Experiments	Jacob Temme/ARL
1700 - 1730	Low Temperature Pyrolysis Pathways	Tony Dean/CS Mines
1730 - 1800	Analysis of Turbulence/LTC Impacts on Ignition	Rainer Dahms/SNL-CRF
1800 - 2000	DINNER	
Low-Temperature Combustion Chemistry Workshop Part 1 – Problems and Challenges, Chair: Ralph Anthenien and Chiping Li		
2000 - 2020	US Army’s Perspectives, Mike Kweon Low-Temperature Combustion Chemistry: Needs and Challenges Relevant to IC Engine	Mike Kweon Ralph Anthenien
2020 - 2030	US Air Force's Perspectives Low-Temperature Combustion Chemistry: Needs and Challenges Potentially Relevant to Future Jet Engines	Chiping Li et.al.
2030 - 2200	Discussion (Participants can request a slot for a presentation and comments of one chart/less than five minutes per person, sent to Ralph Anthenien and Chiping Li via email NLT1900, Monday, Oct 17),	Moderated by Mike Kweon, Ralph Anthenien and Chiping Li
	MEETING ADJOURNED FOR THE DAY	

Agenda Day 4| Monday, October 20, 2016

Time	Title	Speaker
0755 - 0800	Daily Announcements	Stephen Pratt/DOE-ANL, Ralph Anthenien/ARO, Song-Charng Kong/NSF and Chiping Li/AFOSR
Low-Temperature Combustion Chemistry Workshop Part 2 – What we know (existing understanding) and how to solve the problem (innovative solutions), Chair: Ralph Anthenien and Chiping Li		
0800 - 0830	Perspectives on Low-Temperature Combustion Chemistry: Existing Scientific Understanding and Challenges (discussion lead presentation)	Bill Green/MIT
0830 - 1130	Discussion (Participants can request a slot for a presentation and comment of one chart/less than five minutes per person, sent to Ralph Anthenien and Chiping Li via email NLT1900, Monday, Oct 17), moderated by Bill Green, Ralph Anthenien and Chiping Li	
1130 - 1200	Summary Remarks and Meeting Adjournment	