Second International Workshop on Combustion Chemistry Models of Real Liquid Fuels

June 6, 2016
The Liberty Room
Basic Research Innovation and Collaboration Center (BRICC)
4075 Wilson Blvd., Suite 350 | Arlington, VA 22203

Planning Committee:

Fokion N. Egolfopoulos (Chair, USC), Tianfeng Lu (UConn), Venke Sankaran (AFRL/RQ) and Hai Wang (Stanford)

Invitees:

Gurhan Andac (GE)
Tom Bowman (Stanford)
Tom Bruno (NIST Boulder)
Harsha Chelliah (UVa)
Adam Comer (AFIT)
David A. Davidson (Stanford)
J. Tim Edwards (AFRL)

Ronald K. Hanson (Stanford)
Ez Eldin Hassan (AFRL/RQH)
Graham Goldin (CD Adapco)
Yiguang Ju (Princeton)
Tonghun Lee (UIUC)

Suresh Menon (Georgia Tech)
Thierry Poinsot (CNRS, Toulouse, France)
Brent Rankin (AFRL)
Paul D. Ronney (USC)
David A. Sheen (NIST)
Xinyu Zhao (UConn)

Matthew Billingsley (AFRL Edwards)
Ken Brezinsky (UIC)
Michael Burke (Columbia)
Jackie Chen (Sandia)
Philippe Dagaut (CNRS, Orléans, France)
James Driscoll (UMich)
Christer Fureby (Swedish Defense Research Agency)
Matt Harvazinski (AFRL Edwards)
Matthias Ihme (Stanford)
William Green (MIT)
Robert Kee (CSM)
Epaminondas Mastorakos (University of Cambridge, UK)
Joe Miller (AFRL)
Alexei Poludnenko (NRL)
Mel Roquemore (AFRL)
Vaidya Sankaran (UTRC)
Wenting Sun (GeorgiaTech)

Ralph Anthenien (ARO)
Mohan Gupta (FAA)
Chiping Li (AFOSR)

Pamela Chu (NIST)
Wade Sisk (DoE)
Song-Charng Kong (NSF)

Background

The availability of predictive tools for turbulent combustion is of paramount importance to the improvement of efficiency, operability and reliability, as well as to the control and reduction of emissions from modern engines. Proper use of these tools will greatly reduce the time and cost for combustor design and optimization. The combustion process in engines is controlled largely by the couplings of fluid mechanics and chemical kinetics. Reliable combustion simulations require the use of accurate chemistry models for real, multicomponent fuels with compact sizes, but still being capable of capturing all relevant phenomena.

The approach of surrogate fuels has been the dominant paradigm of detailed chemistry model development for over a decade. The approach has been applied to gasoline, jet, and diesel fuels with the number of surrogate components as few as two and as many as twelve. As an indirect approach, a specific surrogate fuel formulation usually has significant difficulties to capture all relevant, important physical and chemical properties of the real fuel. Meanwhile, combustion kinetic models of surrogate fuels invariably are comprised of too many species and reactions to be used for turbulent combustion simulation. The large number of parameters also introduces many assumptions, most of which cannot be verified experimentally and will not be verified theoretically or experimentally in a foreseeable future.

Recently, an alternative approach, called HyChem, was formulated and adopted in several national jet fuel combustion initiatives. HyChem built on the experience, knowledge, and lessons (both positive and negative) garnered in surrogate and other types of model development efforts. The concept is based on physics-based arguments and relies on advanced experimental diagnostics to map the pathways of real fuel decomposition to a handful of small, intermediate species. When combined with detailed chemistry models of foundational fuels, the approach is shown to produce reaction models that are accurate for a wide range of real jet-fuel combustion properties. Built upon on the most important and relevant reaction pathways, this approach also has the advantage of being able to generate models sufficiently compact for modern CFD computations. Recent studies showed that the models resulted using this approach can be reduced to about 25 species to capture ignition, propagation, and extinction of real jet fuel flames, and when the reaction model is combined with DNS, the results show interesting physics that have not been fully recognized or studied previously.

Aims and Goals of the Proposed Workshop

Preliminary reaction models for a quite wide range of real fuels are now available. They include jet fuels (kerosene & JP10), rocket fuels (RP2), and some bio-derived aviation fuels. Some have been tested in CFD codes over a limited range of conditions. The primary theme of this workshop is to address issues relevant to turbulent flame simulations in real engines burning real fuels with realistic chemistry. Discussion will include, among others, CFD implementation, mechanism reduction, and numerical stiffness reduction.

It is apparent that the success of this promising chemistry effort depends on the input from experts with diverse backgrounds and expertise. Finally, the scope and participation will increase notably in the near future with extensive international participation. More specifically, the workshop will be held at the 37th International Symposium on Combustion (Dublin Ireland) in 2018.

Schedule:

Morning – Chemistry Experiments and Models

8:25-8:30	Announcements
8:30-8:45	Welcome remarks and workshop objectives (Egolfopoulos & Li)

Chair: Fokion N. Egolfopoulos

8:45-9:15	Overview of experimental and modeling approaches and results (Wang)
9:15-9:45	High-pressure shock-tube studies of real fuel pyrolysis and oxidation (Brezinsky)
9:45-10:00	Coffee Break
10:00-10:15	New shock-tube facility at Georgia Tech (Sun)
10:15-10:45	Jet stirred reactor study of real fuel oxidation (Ronney)
10:45-11:15	Mechanism reduction (Lu)
11:15-11:45	Direct numerical simulations of high-speed combustion (Poludnenko)
11:45-12:00	Open discussion

Afternoon – CFD implementation

Chair: Hai Wang

1:00-1:30	Large-eddy simulation of turbine combustion (Poinsot)
1:30-2:00	Turbulent combustion research at Cambridge (Mastorakos)
2:00-2:30	Detailed chemistry in CFD (Goldin)
2:30-3:00	LES simulation of real-fuel combustion in turbine engines (Menon)
3:00-3:15	Coffee Break
3:15-3:45	LES simulation of real-fuel combustion in turbine engines (Ihme)
3:45-4:15	Overview of simulation of high-speed combustion (Sankaran)
4:15-5:00	Open discussion