Summary of States/Plans of Flame DWG

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Goal: Develop models and predictive tools for turbulent combustion modeling

Fuel: Burning properties
Egolfopoulos, Ju, Law

Fuel: Emission properties
Egolfopoulos, Law

Kinetic mechanism validation
Egolfopoulos, Ju, Law

Flame theory/Modeling
Ju and Law

Turbulence-Combustion Modeling
(DNS/LES/PDF)
Chen & Pope
Fuel burning properties and mechanism validation: Status

• **Fuel burning Properties (C₀-C₂ foundation fuels):**
  – Flame speeds, ignitions, and extinction limits of H₂/CO/CH₄/C₂H₄/C₂H₆ mixtures were obtained
  – Large uncertainties of existing mechanisms at high pressure (HO₂ related reactions and the third-body collision efficiency)
  – Results led to a new high pressure mechanism development

• **Oxygenated fuels**
  – Flame speeds and extinction of methyl-esters, alcohols, aldehydes, and ketones are measured. It was found that the size of methyl esters affects the flame speed and extinction limit.
  – Flame structure for t-butanol is measured, sub-models of intermediate species significantly affected the extinction limits
  – Led to an improved methyl-ester mechanism development.
Fuel emission properties: Status

- **Soot and NO$_x$ emissions of methyl esters**
  - Soot and NO$_x$ emissions of saturated and unsaturated methyl esters and biodiesel/diesel blends were studied.
  - The unsaturated bonds increased the sooting propensity.
  - Adding biodiesel to diesel significantly reduced the extent of soot formation.
Flame theory and modeling: status

- **Correlation for diffusion flame extinction: chemistry and transport**
  - A generic correlation for diffusion flame extinction using radical index and transport-weighted enthalpy is developed.
  - The method allows extraction of flame chemistry information by decoupling the transport effect from the kinetic effect.
  - The method demonstrates the reactivity similarity between methyl decanoate and methyl butanoate.

- **Low temperature ignition**
  - Low temperature ignition of n-heptane is modelled in both steady and unsteady counterflow diffusion flames.
  - NTC effect and multi-stage ignition are observed at elevated pressure.
  - Flow and species fluctuations increase flow/chemistry coupling and dramatically changes the ignition delay time.

- **Turbulent premixed combustion regime diagram**
  - The boundaries of the standard turbulent premixed combustion regime diagram were modified by introducing the influences of flame instability.
Turbulent combustion: status

• Turbulent flame experiments
  – Experiments of turbulent expanding flames at elevated pressure were conducted and some preliminary results are obtained.
• Development of LES/PDF/ISAT method for turbulent combustion modeling
  – LES/PDF/ISAT methodology being developed.
  – The method enables the computationally-efficient implementation of the chemistry of transportation fuels.
  – Model calculations have been performed for a turbulent piloted CO/H₂ jet flame (Sandia Flame E) studied at Sandia using direct numerical simulation (DNS).
• Petascale direct numerical simulations
  - 3D DNS of turbulent HCCI in inhomogeneous mixtures were conducted.
  - The effect of stratification on the presence of spontaneous ignition and deflagration waves in multi-stage ignition.
  - A new method was developed to identify accurate low-dimensional manifolds (LDMs) embedded in high-dimensional (in phase space) turbulent combustion data using a novel technique based on Isomap.
Fuel burning properties: Challenges and plan

- High pressure global flame properties for $\text{C}_1$-$\text{C}_4$ foundation fuels, oxygenated fuels, and intermediate stable species to fill the gap of mechanism validation.
- High pressure burning properties with H2O/CO2 dilution (kinetics, EGR, and third-body effect).
- Develop new diagnostic approaches for the measurements of important intermediate and radical species in flames to constrain the kinetic coupling between chemistry and transport.
Flame theory/modeling

Challenges and plan

• Is there any comprehensive correlations between global flame properties, transport, and radical index for oxygenated fuels and premixed flames.

• Understand quantitatively chemistry and transport (convection and diffusion) interaction in high pressure non-premixed flames.

• Reduce the uncertainties in flame speeds and extinction limit experiments.
Turbulent combustion: Challenges and plan

• Conduct higher pressure turbulent flame studies by incorporating the DL instability.
• Completion of the implementation of the LES/PDF/ISAT methodology on large-scale computer systems.
• Use the HCCI DNS data to evaluate and improve combustion and mixing models for RANS and LES.