Summary of States/Plans of Flame DWG

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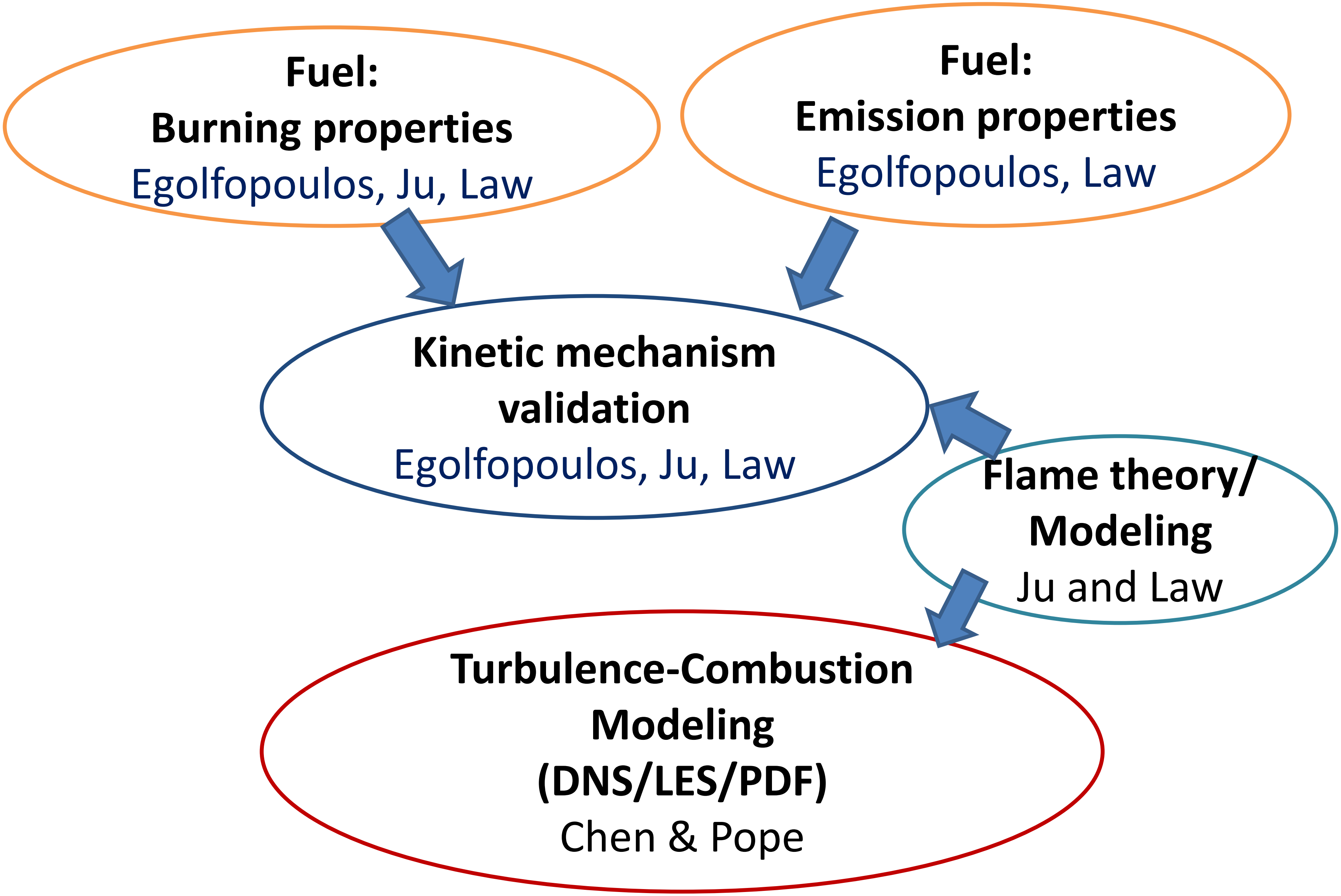
Goal: Develop models and predictive tools for turbulent combustion modeling



Fuel burning properties and mechanism validation: Status

- **Fuel burning Properties (*C_0-C_2 foundation fuels*):**
  - Flame speeds, ignitions, and extinction limits of $H_2/CO/CH_4/C_2H_4/C_2H_6$ mixtures were obtained
  - Large uncertainties of existing mechanisms at high pressure (HO_2 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/H_2 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 C_1-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.