

## Fuel Chemistry and Chemical Kinetics: Capabilities and Services

### Expertise

- Combustion Design & Dynamics
- Combustion Modeling & Problem Analysis
- Fuel Efficiency
- Emissions Reduction
- Particulate Control
- Fuel Chemistry
- Fire Safety
- Fire Investigation
- Explosion Analysis

### Industries

- Utilities
- Oil & Gas
- Chemical & Industrial Process
- Aviation & Defense
- Manufacturing

### Experimental Facilities

- *Flow Reactor*: Ignition-delay time
- *High-Pressure Burner*: Blow-out and emissions measurements
- *Atmospheric Pressure Test*: Rigs with air flow to 0.5 kg/s
- *CEMS*: CO, CO<sub>2</sub>, NO<sub>x</sub>, O<sub>2</sub>, and THC
- *GC-MS and GC-BID*: Hydrocarbon species measurements
- *Spectrometers*: FTIR and Visible/UV

Please contact us to discuss your project requirements

www.csefire.com  
info@csefire.com  
(410)-884-3266

**Combustion Science & Engineering, Inc.**  
8940 Old Annapolis Road  
Suite L  
Columbia, Maryland 21045  
USA

### Detailed fuel chemistry for a wide variety of fuels

- Natural gas, LNG, jet fuels, renewable jet fuels, solid fuels
- Includes low-temperature oxidation reactions, vitiated combustion kinetics, and full nitrogen chemistry (for NO<sub>x</sub> prediction under ultra-lean conditions)
- Validated for ignition flame speed and emissions against experimental data

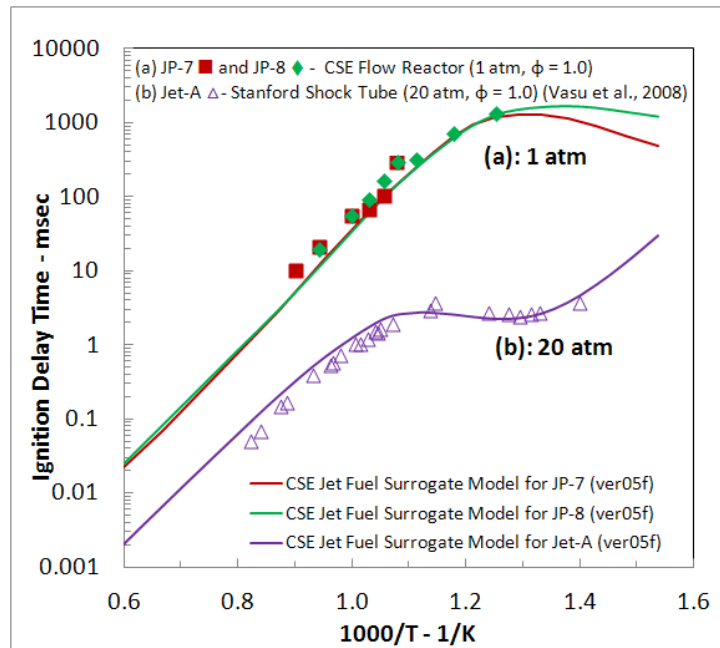


Figure 1. CSE detailed surrogate kinetic mechanism for jet fuel combustion compared with ignition delay time data

### rkmGen™ – Proprietary optimization package for reduced chemical mechanisms

- Size of the mechanism (number of reactions) may be user-specified
- Optimized against target data that may include ignition delay time, blow-out, flame speed, and emissions
- Suitable for CFD simulation of gas turbine combustors, augmentors and scramjets to predict flame instability and emissions

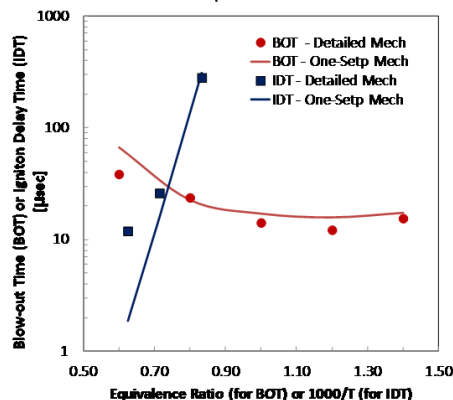


Figure 2. One-step ethylene kinetic model predictions for ignition (IDT) and blow-out (BOT) compared with GRI-3.0 mechanism

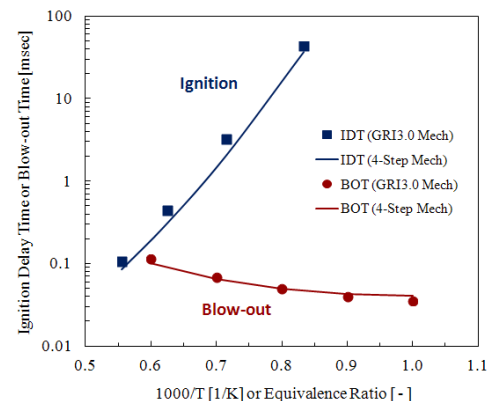


Figure 3. Four-step global mechanism for methane optimized for ignition and blow-out

### 1-D models of fuel transformation from pre-heat to combustion

- Physical models for multi-component evaporation of real fuels such as Jet-A, diesel, etc.
- Chemical kinetic models for pyrolysis and combustion
- Chemical reactor network models for emission (e.g., NO<sub>x</sub> and CO) analysis using detailed chemistry

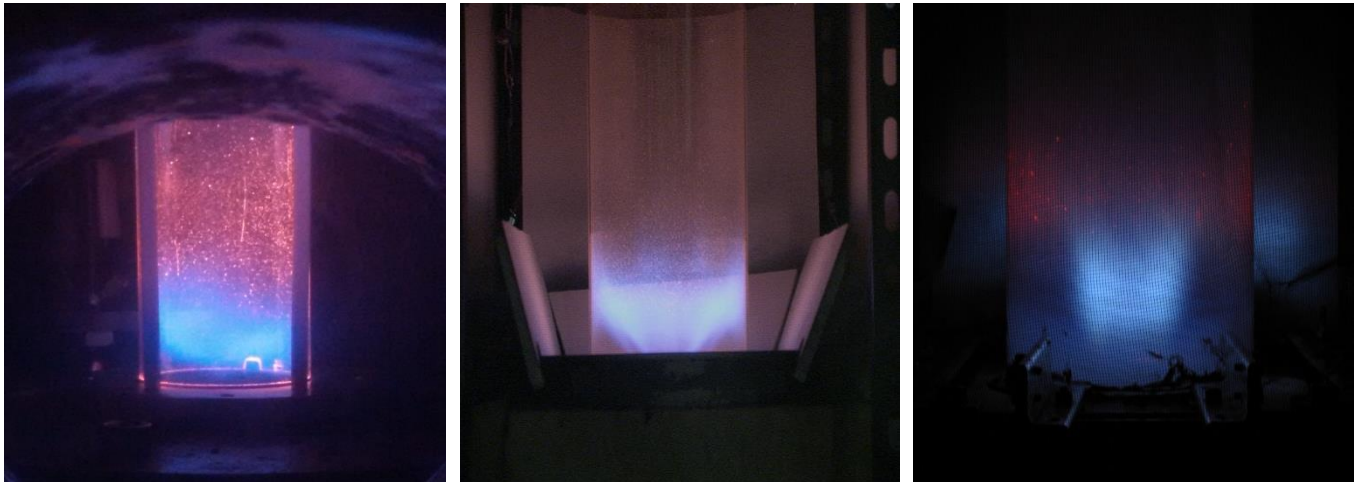


Figure 4. Measurements of pollutant emissions from premixed flames in CSE's laboratory

### Detailed kinetic models for fuel pyrolysis (thermal cracking) and oxidative cracking

- Prediction of gas-phase and surface-phase deposition
- Prediction of low temperature fuel modification and particulate formation

### Extensive Experimental Facilities (see side bar)

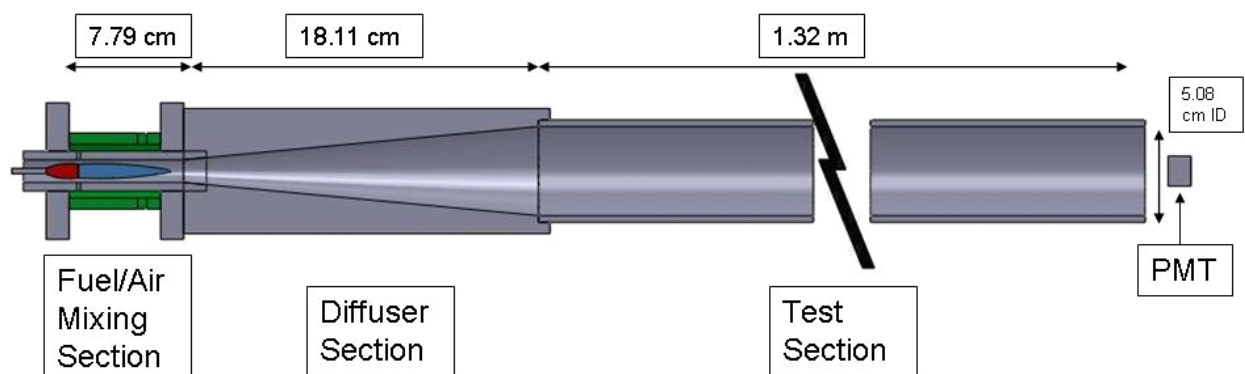


Figure 5. Schematic of CSE flow reactor facility for ignition delay time measurements