Combustion at High Pressure

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Introduction & Motivation

❖Current chemical models for combustion consist of kinetic data for thousands of reactions. These models are validated through detailed comparisons with wide ranging experimental observations of flame properties. Unfortunately, much of the validation data is for low pressures (e.g., 1 bar), whereas combustion devices are generally operating at much higher pressures (e.g., 100 bar for many advanced engine concepts).

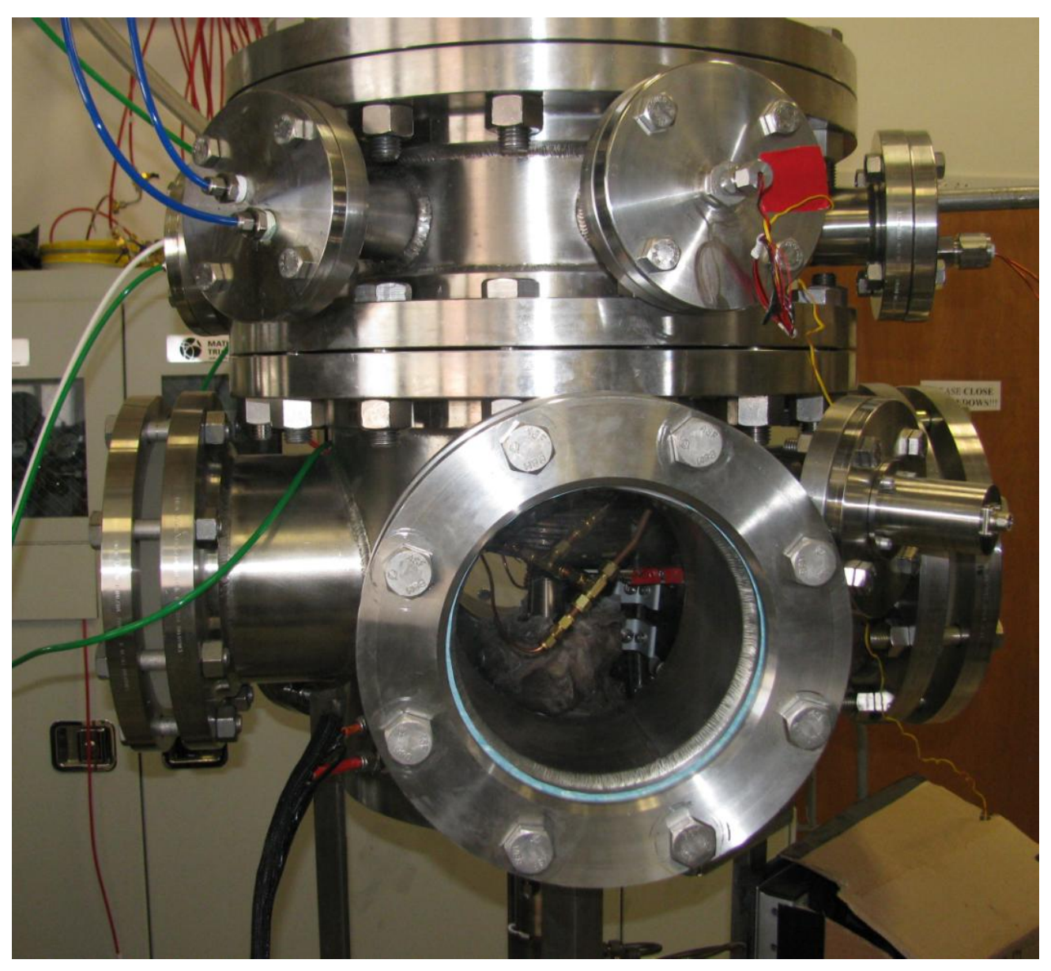
❖Recent studies have demonstrated great shortcomings for even the best chemical models at high pressure. The CEFRC is addressing these shortcomings through the generation of wide-ranging validation data at significantly higher pressures and the use of this data in the development of improved chemical models. In particular, we are developing and applying methods for studying ignition, propagation, and extinction in stagnation and spherically expanding flame configurations, flame properties for turbulent flames, ignition delays and multi-species time histories in both rapid compression machines and shock tubes, and elementary rate coefficients in shock tubes.

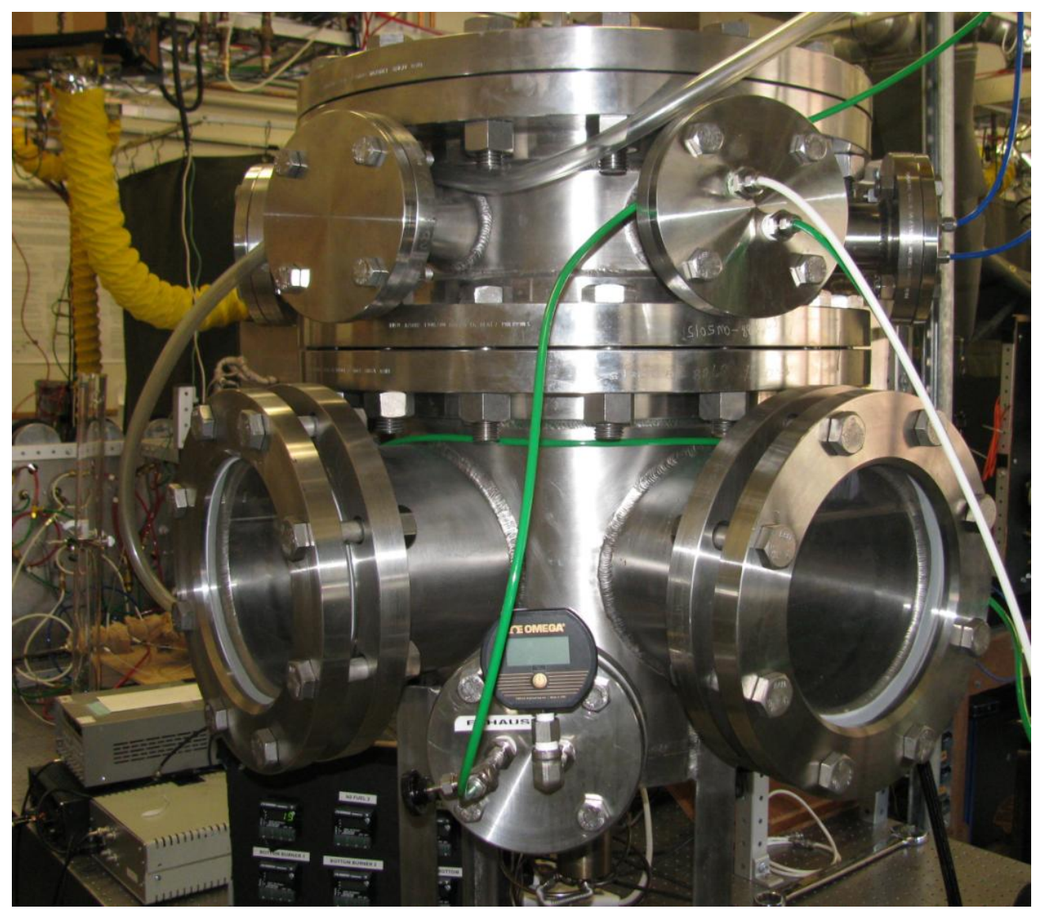
❖All of these measurements are being performed for pressures ranging up to 20 to 40 bar, with an initial focus on butanol combustion as a key prototypical biofuel. The combination of modeling and theoretical reaction kinetics is being used to improve the chemical model for butanol combustion through careful theoretical studies of the key chemical reactions as indicated by the modeling.

Ignition and Extinction Studies of Stagnation Flames

Use of a New State of the Art High Pressure Chamber

- Pressure range: 0.5 to 20 bar
- Fuel types: gaseous as well as light and heavy liquid fuels
- Diagnostics:
  - » Thermocouple for temperature measurements
  - » Digital particle image velocimetry (DPIV) for fluid velocity measurements





Constant Volume Ignition and Propagation Flame Studies

Use of a New Constant Volume Chamber

- Pressure range: 0.5 to 40 bar
- Fuel types: gaseous and light liquid fuels
- Ignition: Combination of traditional and novel approaches
- Diagnostics: Combination of traditional and novel approaches to track the flame-front and characterize the state of ignition

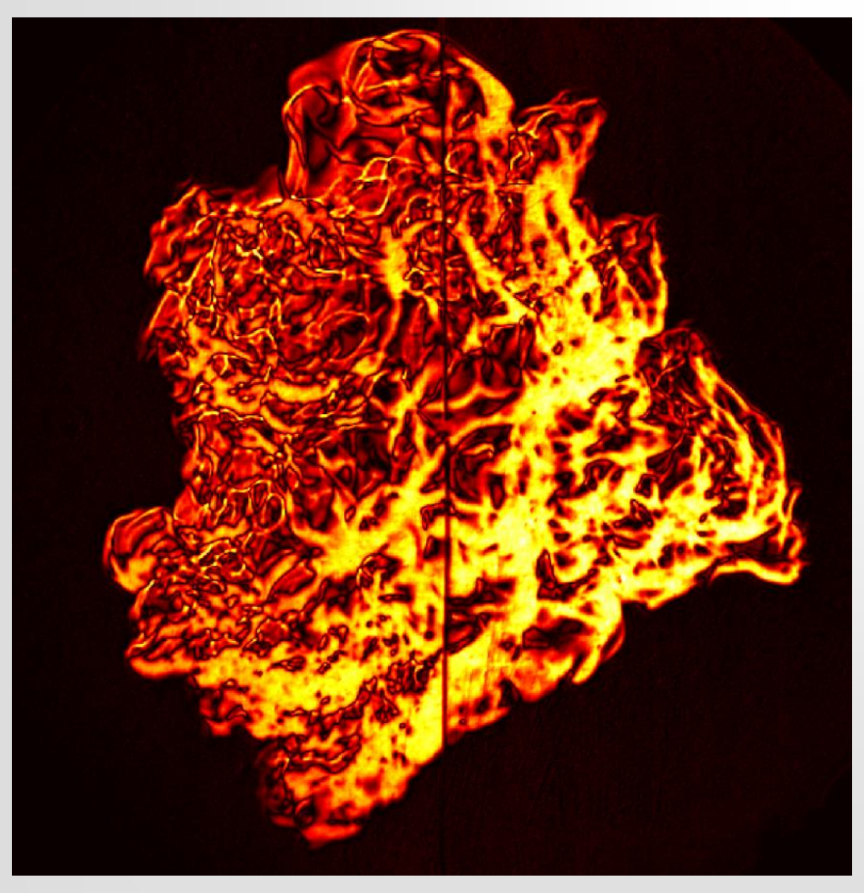
Turbulent Flames at Elevated Pressures

Effects of increasing pressure on the structure & propagation of turbulent flames:

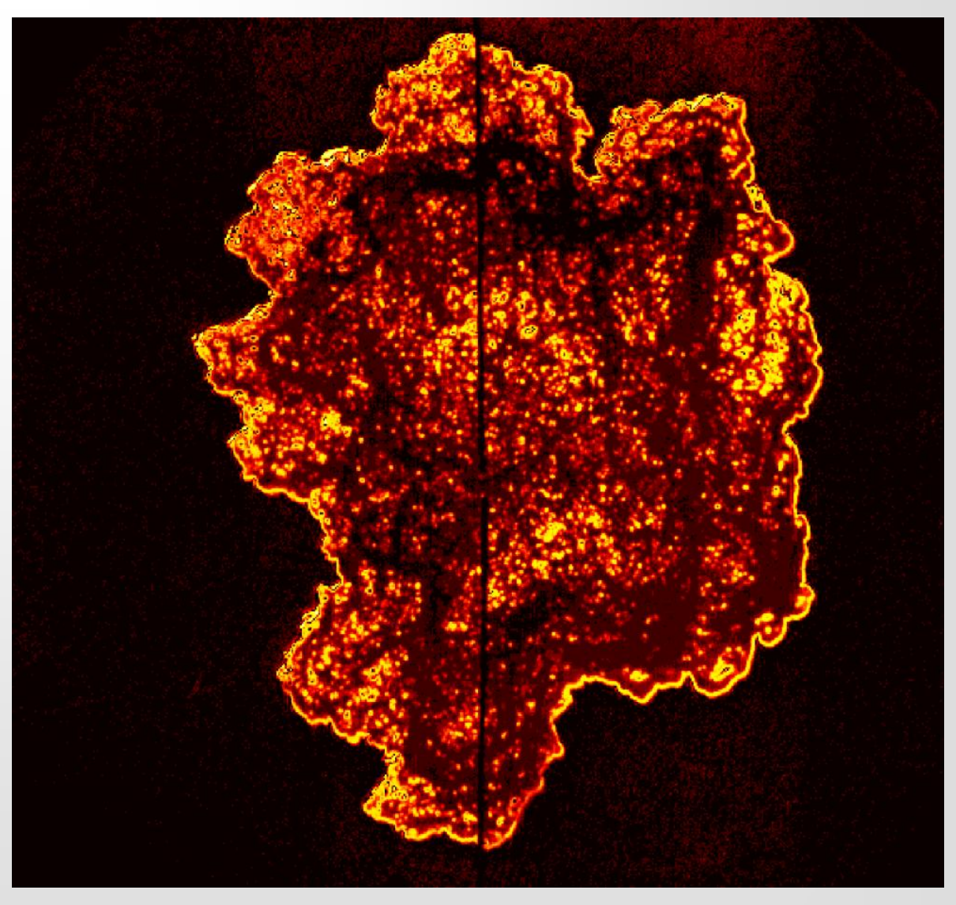
- – Appearance of fine structure
  - Reduced thickness of embedded flamelets due to increased chemical reactivity
  - Reduced thickness further triggers instability-induced wrinkling of the flamelets
- – Burning rate is increased
  - Increased chemical reactivity
  - Increased flamelet surface area due to wrinkling

Images of Turbulent Premixed Methane-Air Flames

Pressure: 1atm



Pressure: 5atm

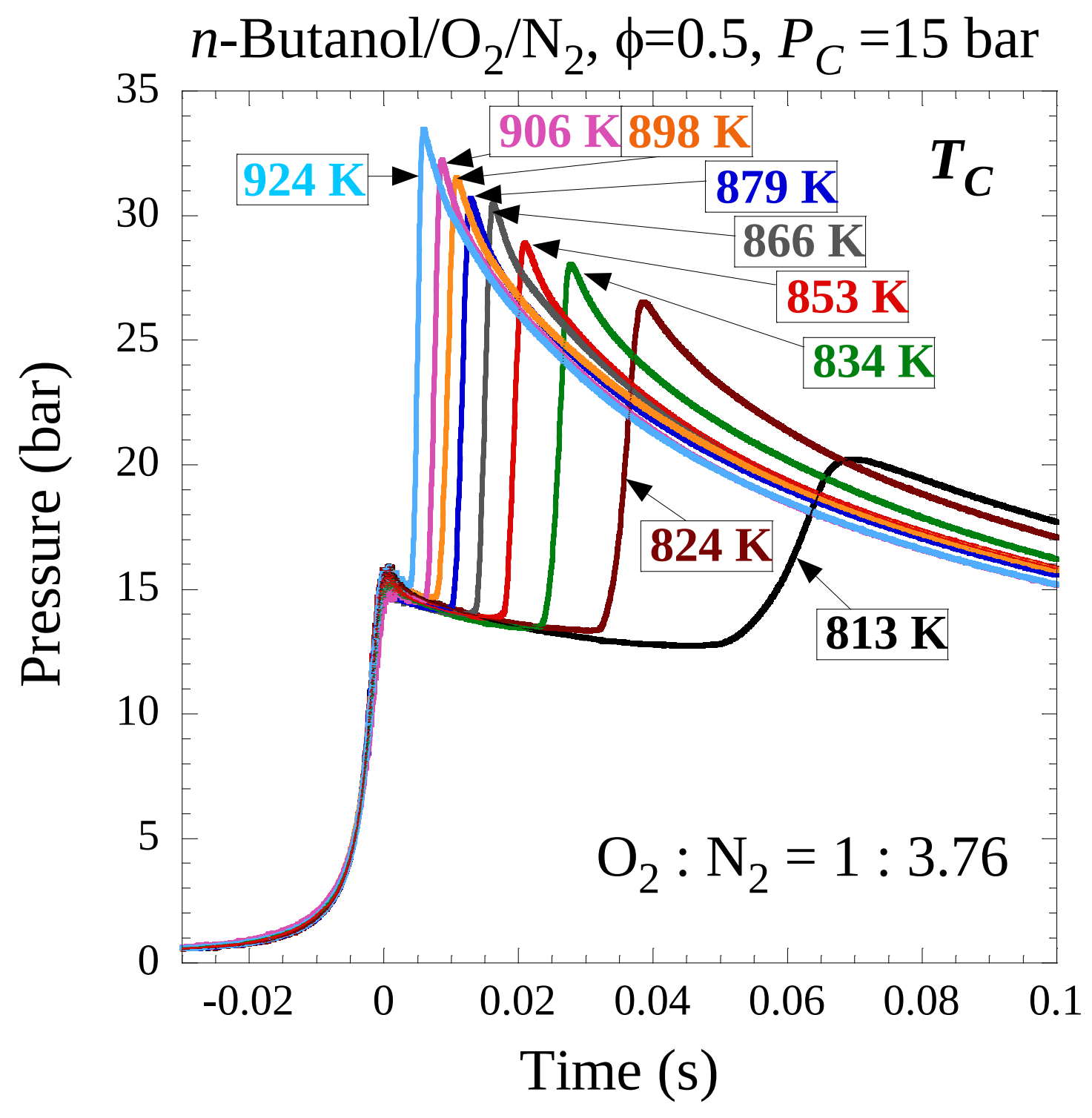


Increase in pressure reduces flame thickness and triggers flame wrinkling at progressively smaller scales

Autoignition of Biofuels

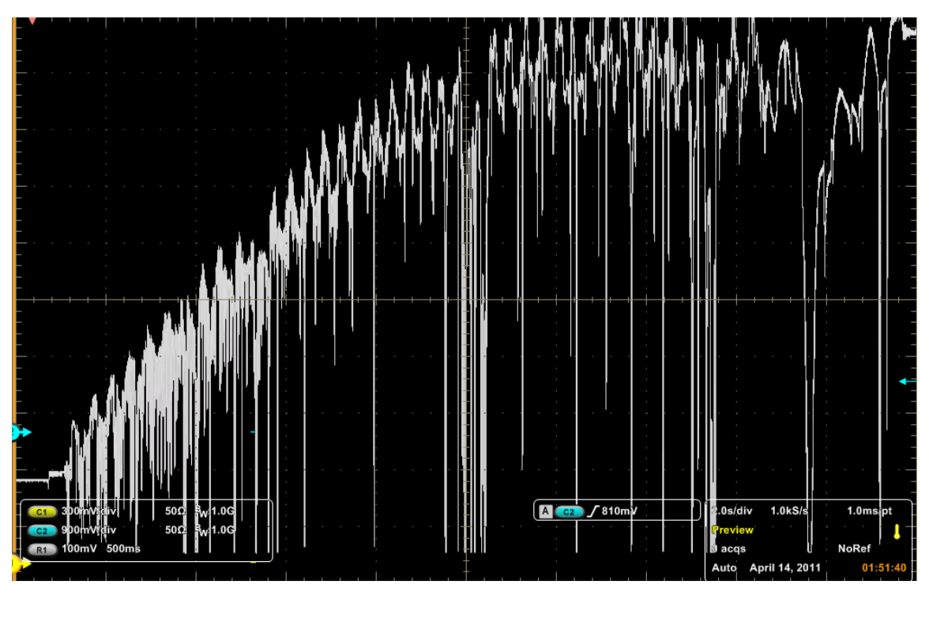
Rapid Compression Machine

A Rapid Compression Machine is used to study the autoignition trends of biofuels, including the isomers of butanol and iso-pentanol



In-situ Measurements of Combustion Intermediates

- Mid-IR Quantum Cascade Lasers are used to study the time-resolved concentrations of CO and H_2O_2 in the Rapid Compression Machine
- These data provide important information about the progress of the combustion process

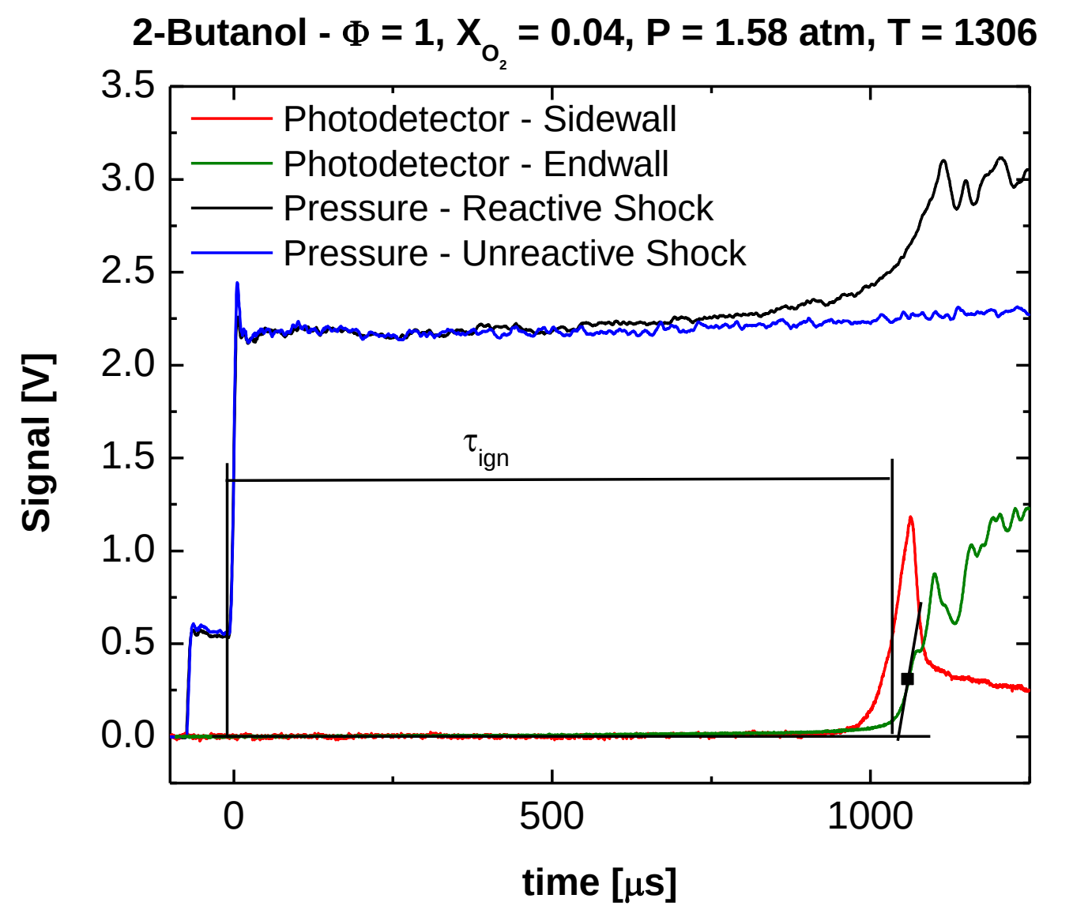


Signal transmitted through test cell containing H_2O_2

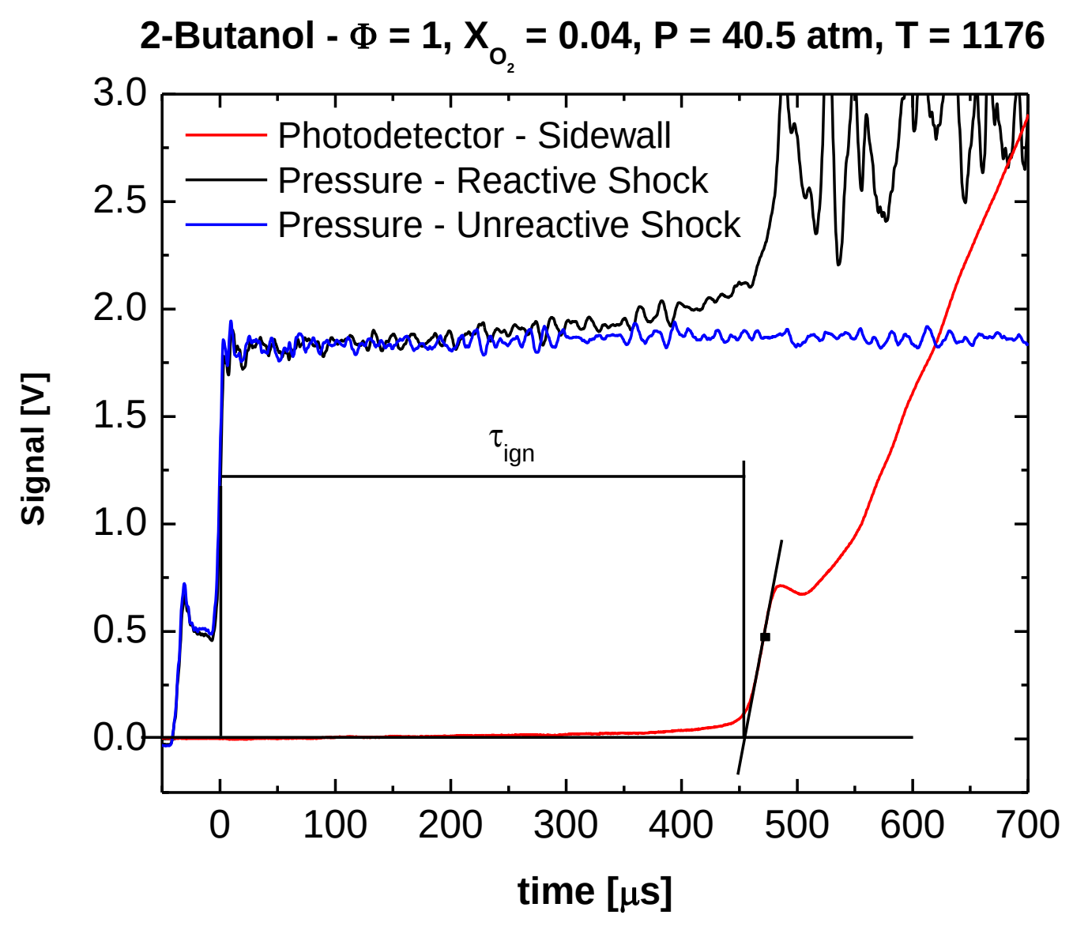
Shock Tube Butanol Ignition Measurements

Example Low and High Pressure Data

- Ignition delay time measurements using pressure and OH* emission
- Low-P experiments have small facility effects (dP/dt~0%/ms to 500ms, 1%/ms to 1.0 ms)



- High-pressure experiments have negligible facility effects: (dP/dt~0%/ms) to 2 ms
- Near-constant-volume performance allows zero-dimensional CHEMKIN modeling

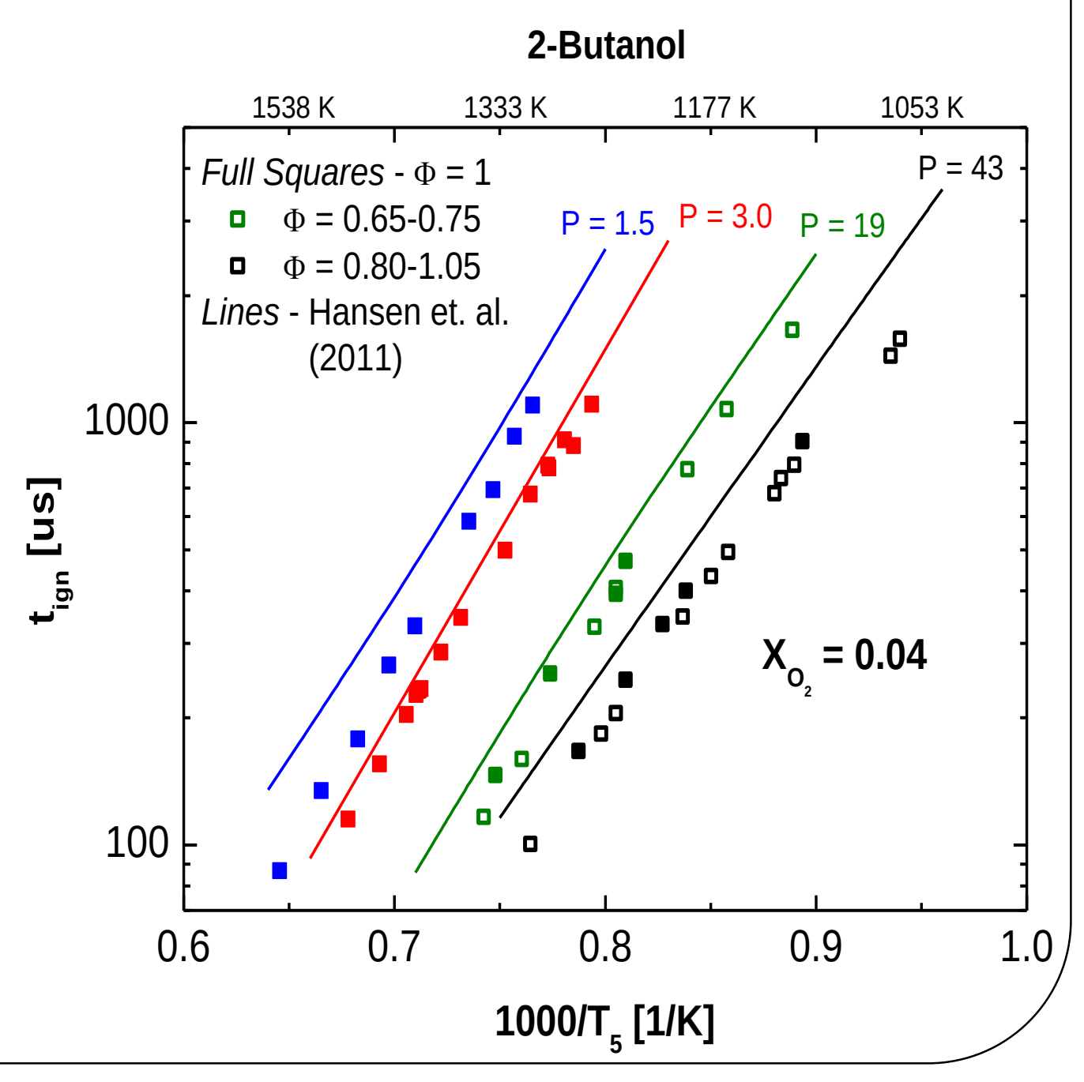


Butanol Isomers

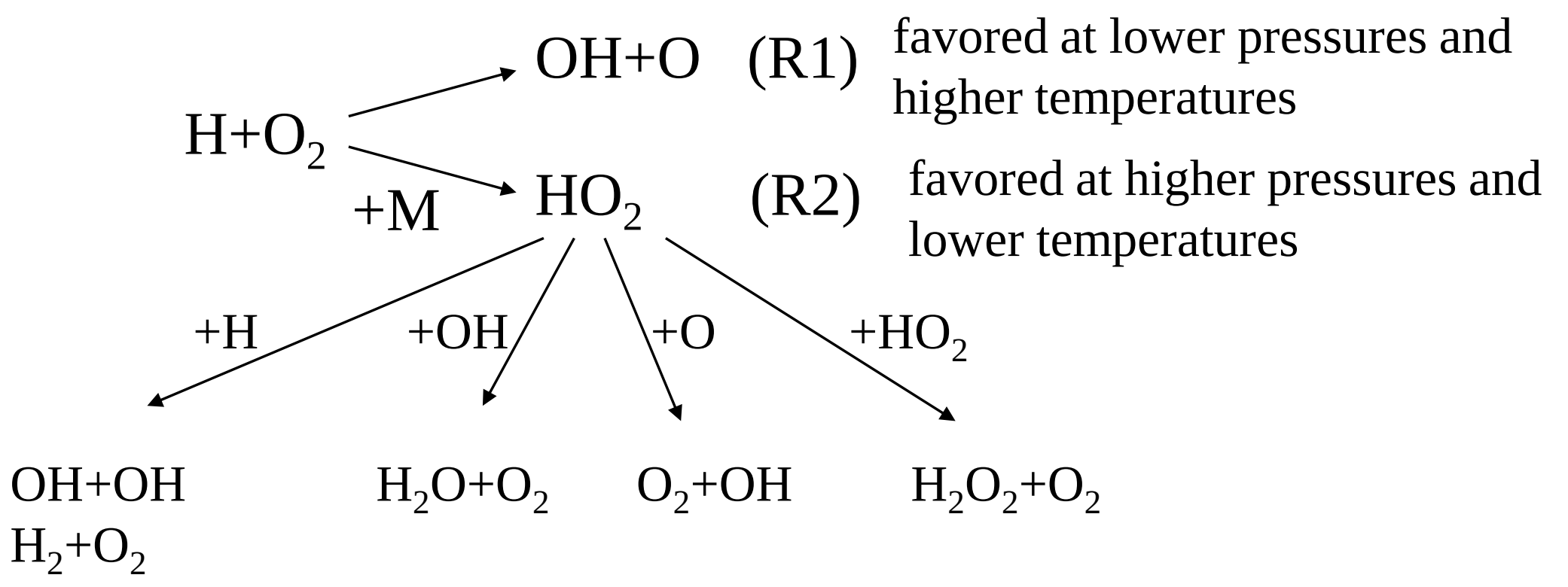
Ignition delay times (IDT) measured for all butanol isomers: 1.5 to 43 atm

IDT scales as $P^{-(0.6-0.8)}$ depending on the isomer and conditions

High quality data will allow refinements to Hansen et. al. (2011) mechanism



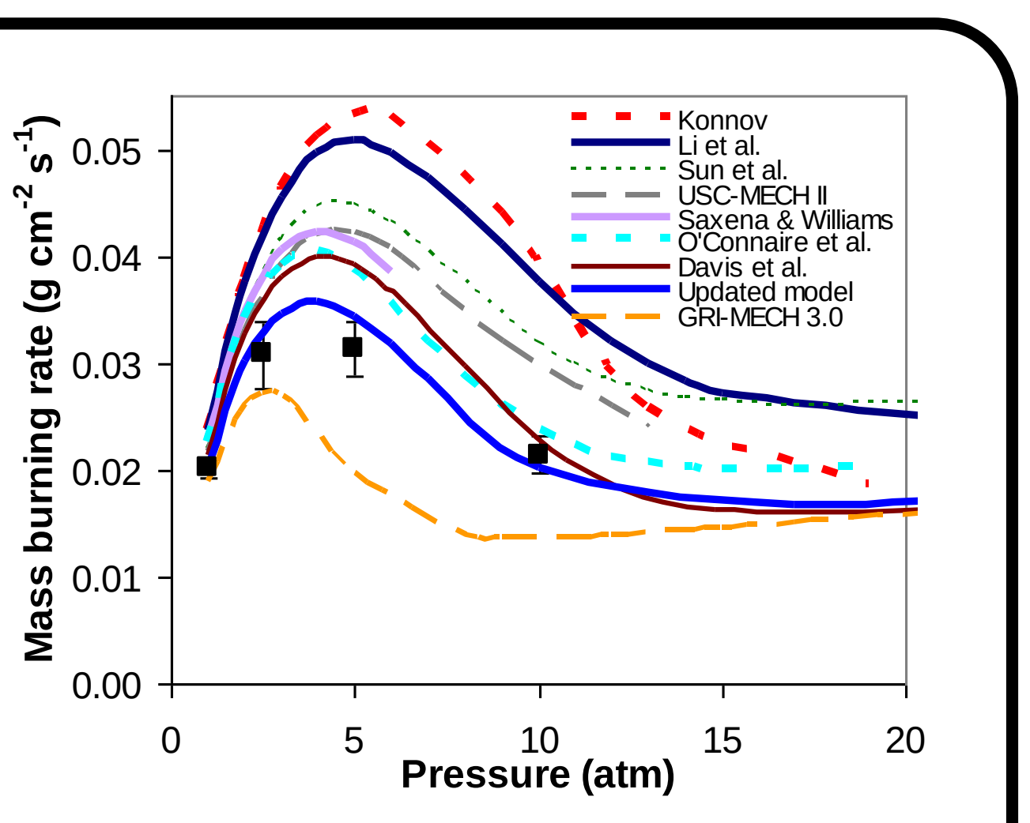
High Pressure Burning Rates and Kinetic Assessment of Mechanisms

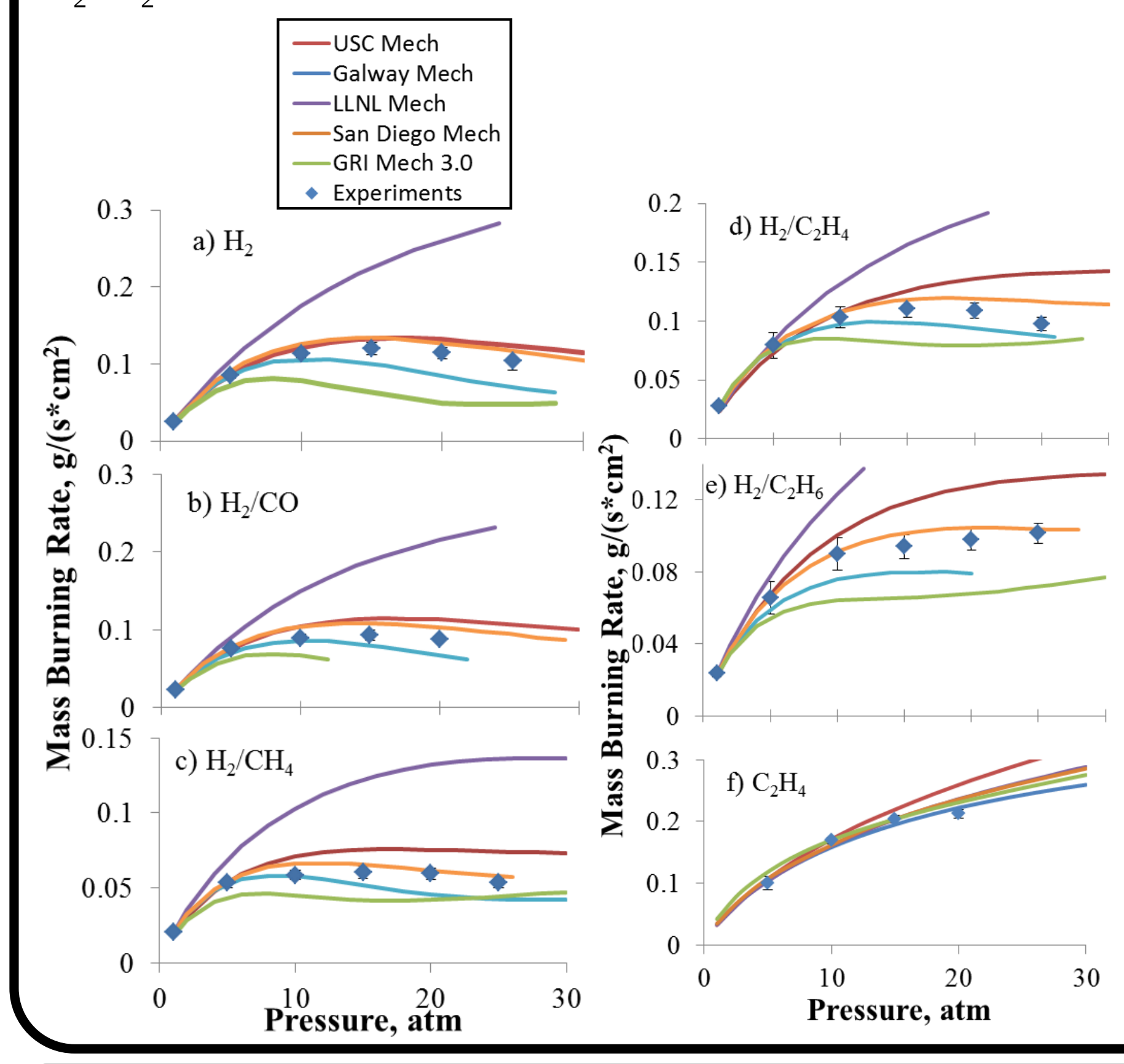


$H+O_2 \rightarrow OH+O$ (R1) favored at lower pressures and higher temperatures

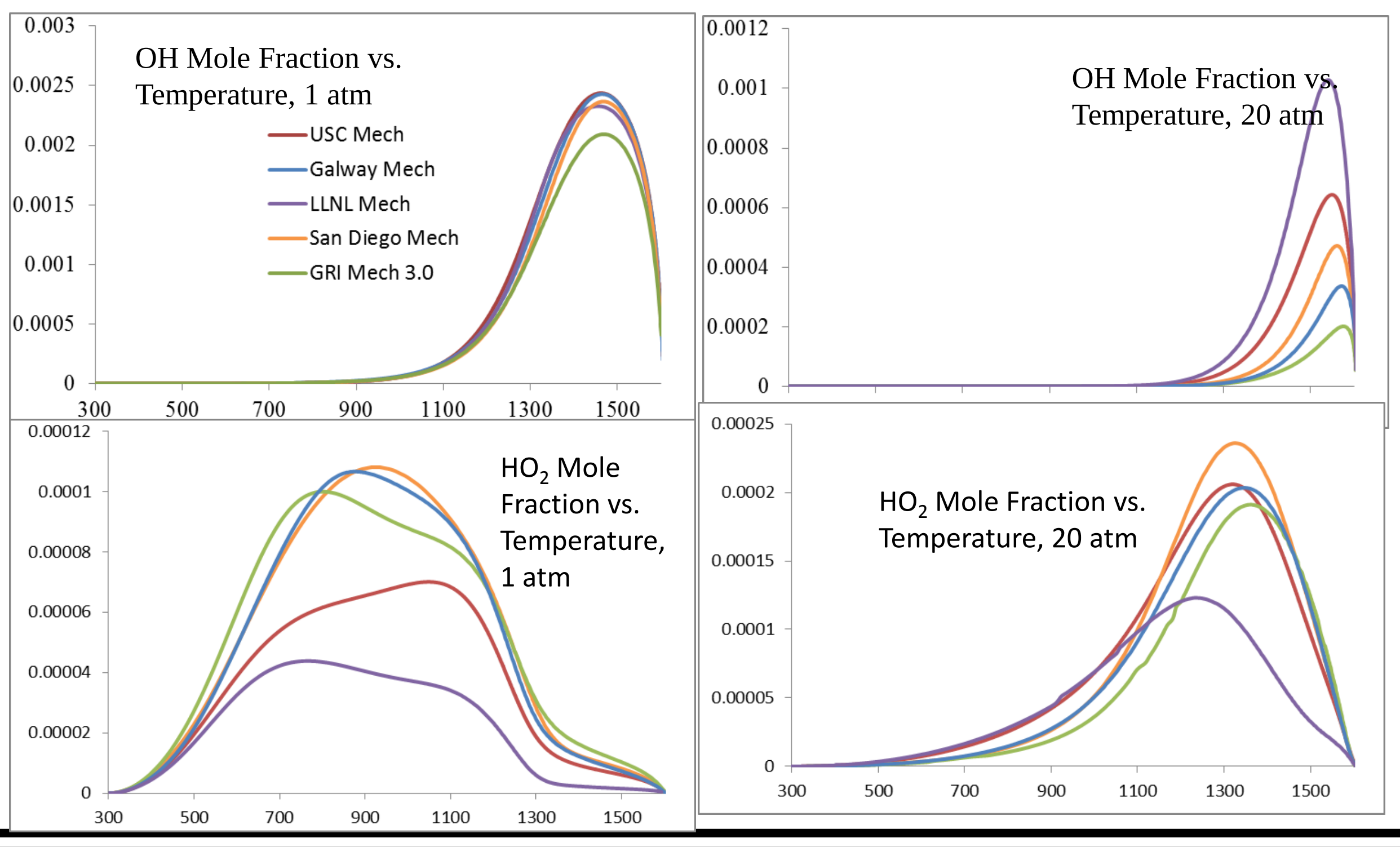
$H+O_2 \xrightarrow{+M} HO_2$ (R2) favored at higher pressures and lower temperatures

HO_2: +H → OH+OH, H_2+O_2; +OH → H_2O+O_2; +O → O_2+OH; $+HO_2$ → $H_2O_2+O_2$





Effect of Pressure and Model Variation on Radical Profiles – H_2/C_2H_6



Conclusions

Current mechanisms have great uncertainties at the high pressures typical of combustion devices.

- At high pressures the H + O_2 chain branching is taken over by stabilization to HO_2 and the chemistry of HO_2 becomes very important.

Developed and applied methods for measuring key combustion properties at pressures up to 20-40 bar.

- Ignition, propagation, and extinction in stagnation and spherically expanding flame configurations, flame properties for turbulent flames, ignition delays and multi-species time histories in both rapid compression machines and shock tubes, and elementary rate coefficients in shock tubes.

We are using these properties to develop accurate chemical mechanisms for combustion of

1. Core fuels (H_2/H_2CO/CH_3OH/CH_4/C_2H_6/C_2H_4/C_2H_2/CH_3OCH_3, etc.).
2. Biofuels with an initial focus on butanols.

   Using sensitivity analysis to suggest key elementary reactions for detailed theoeretical/experimental study.