NATIONAL ENERGY TECHNOLOGY LABORATORY

NETL Combustion Research

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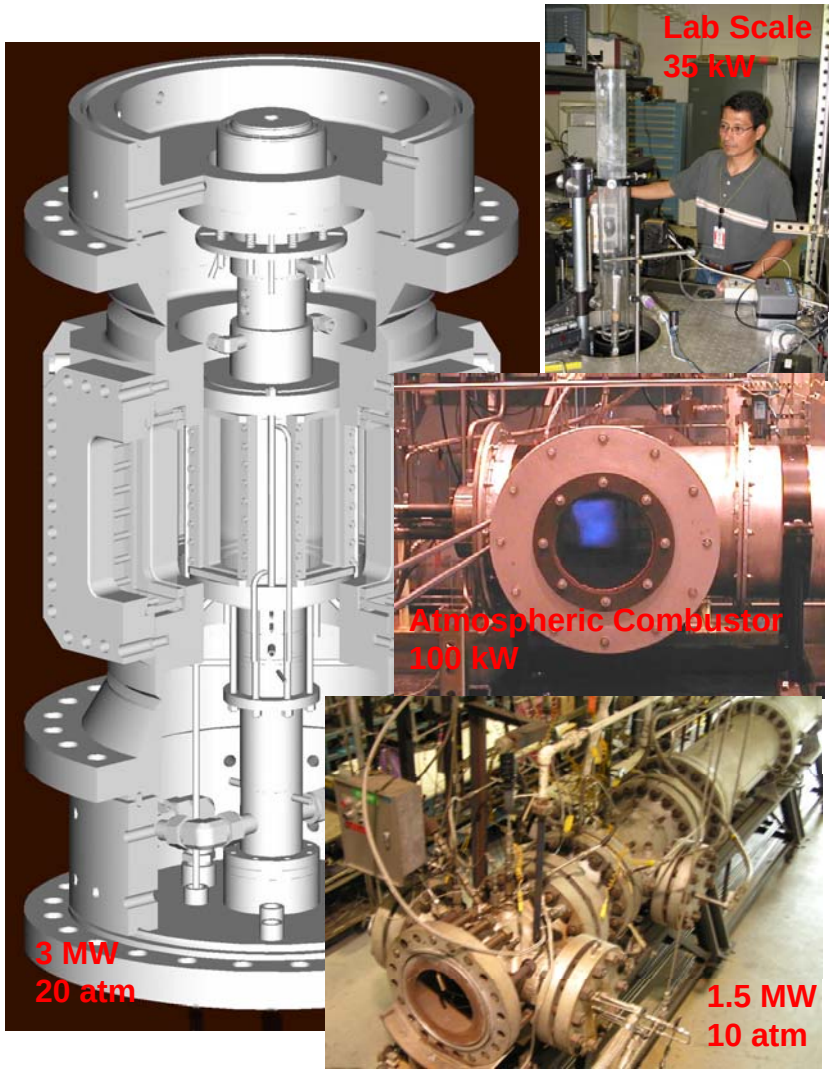
UTSR Workshop Oct. 27-29, 2009, Orlando, FL

Outline

- **Overview of NETL combustion research over the last two years.**
  - NETL combustion facilities.
  - Thickened Flame model development and validation with LSI.
  - Hydrogen dilute diffusion flame studies.
  - Fuel flexibility studies.
  - Combustion dynamics experiments and simulations.
  - Laser diagnostics development.
  - University work.

Combustion Science Team Role at NETL

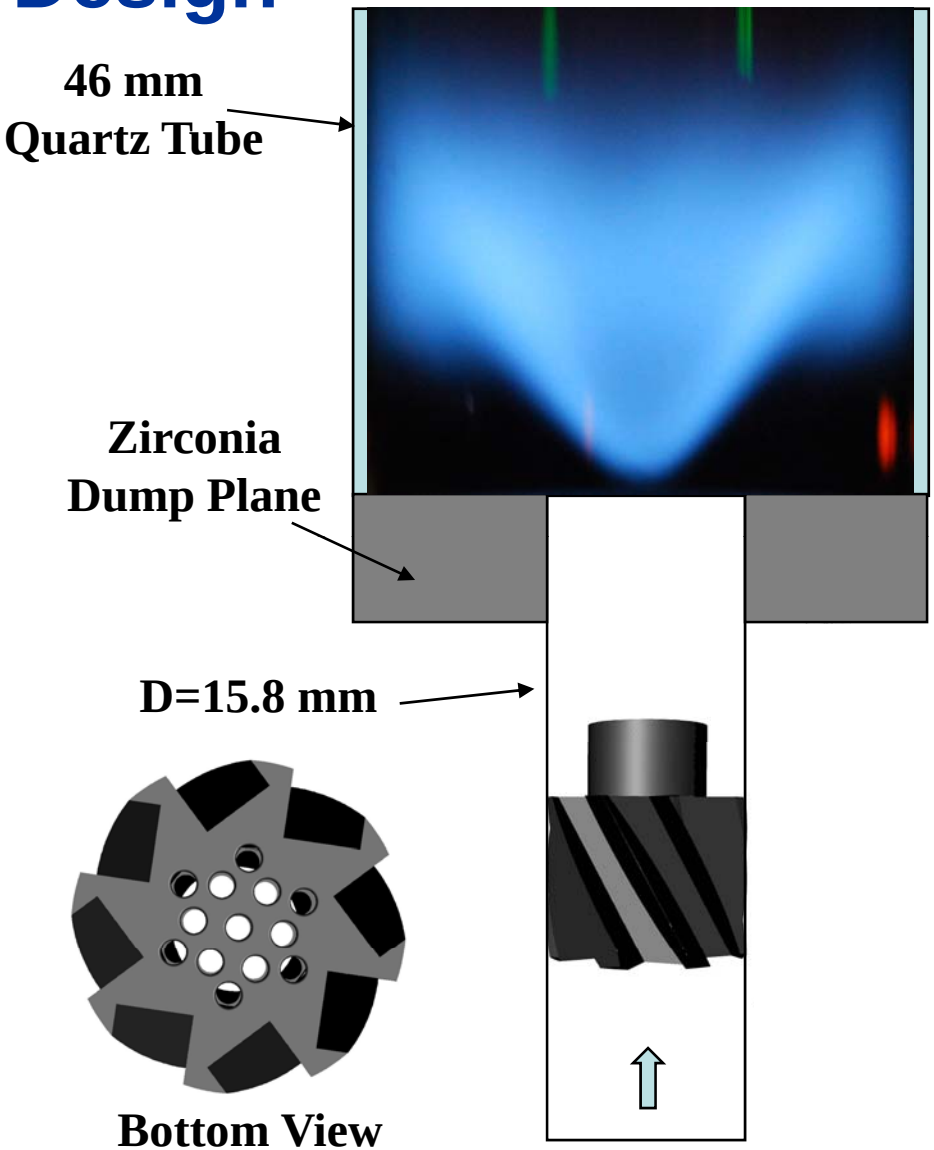
- **Provide a "corporate R&D" function for FE programs**
  - Develop enabling science for turbine technologies
  - Investigate innovative new concepts
  - Bridge the gap between university and industrial-scale R&D with unique facilities
- **Provide technical evaluations to Technology Managers, Project Management, and OEM's**



Thickened Flame Model Development

- **Develop and validate a Thickened Flame (TF) modeling approach for LES of premixed combustion.**
  - Extend previous work to multi-step reactions.
  - Improve sub-grid wrinkling efficiency model.
  - Implement in FLUENT and validate using laboratory scale experiments.
- **Collect validation data in a lab-scale swirl-stabilized premixed combustor.**
  - Develop scaled-down version of the Low-Swirl Burner (LSB).
  - Collect validation data (PIV, OH-PLIF, wall temperature, etc.)

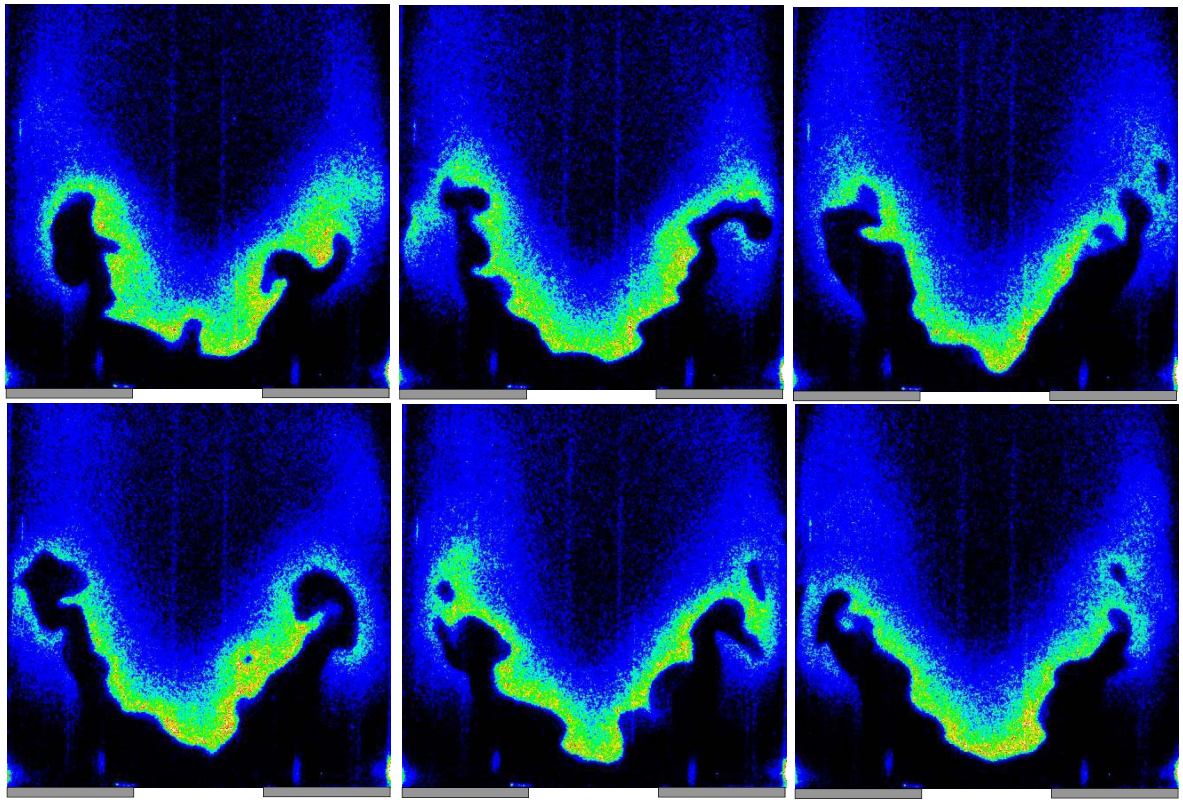
Combustor Design



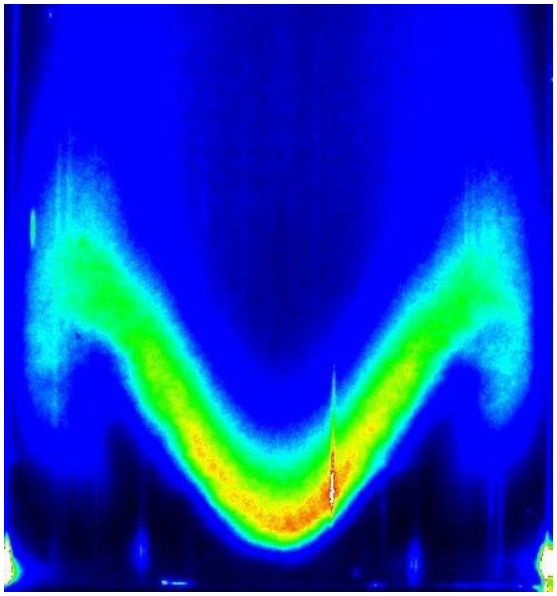
U_{avg} = 3.8 m/s
S_L = 18 cm/s (CH_4/Air, ϕ=0.7)
U' ~ 1 m/s
l_t ~ 6 mm
Re_t = 375
Ka = 1.25

OH-PLIF Imaging

CH_4/Air ϕ=0.70



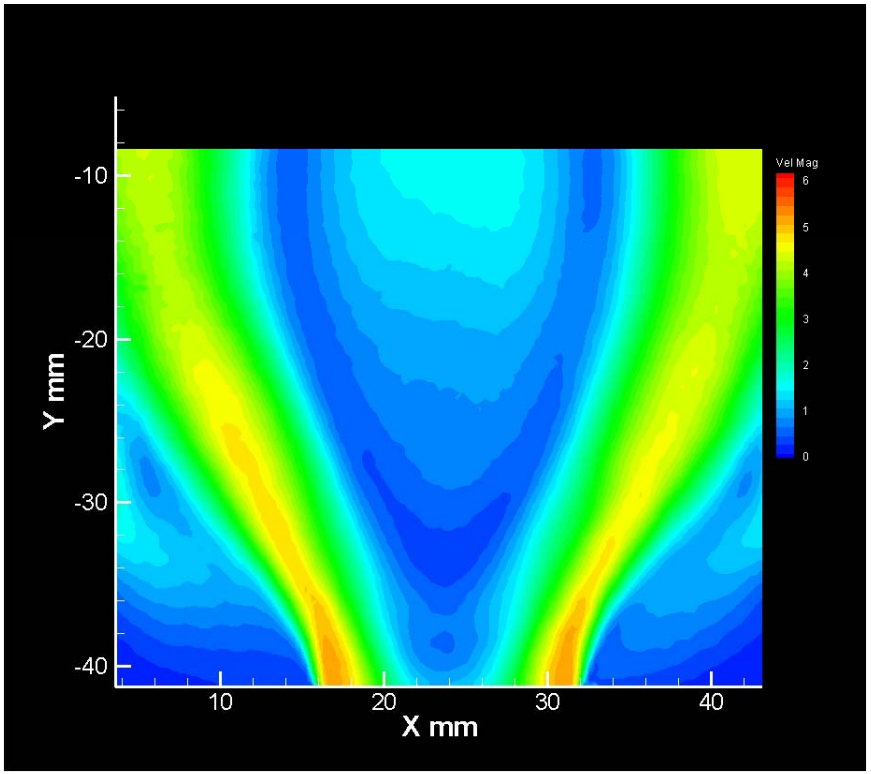
Average of 100 shots



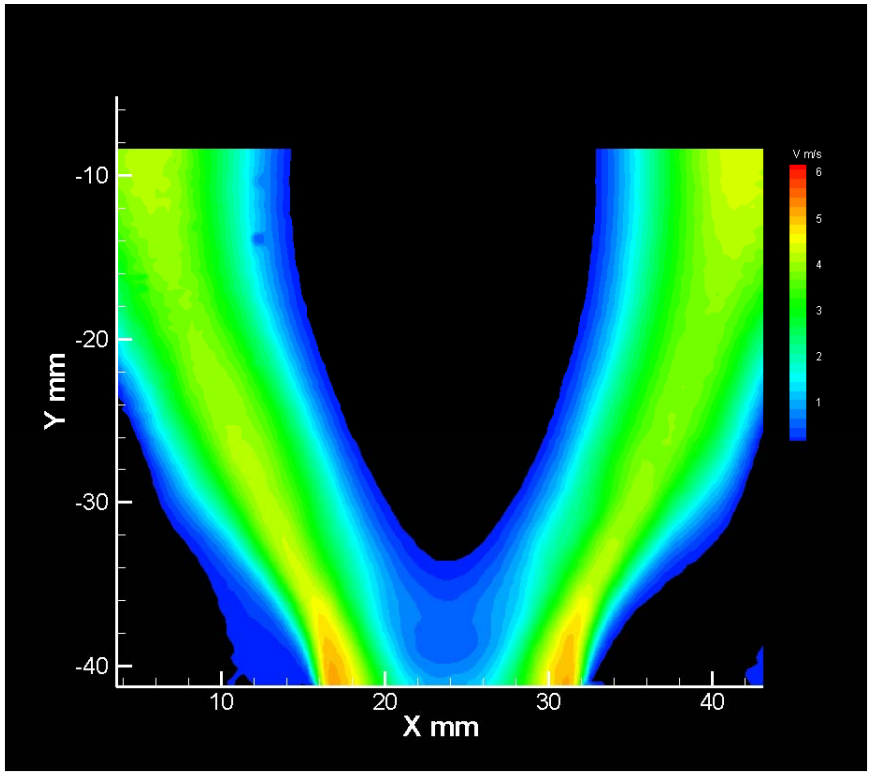
- **Typical bowl-shaped flame**
- **Blow-off at ϕ=0.52**

PIV Results: CH_4 / Air, ϕ=0.7

Mean velocity magnitude

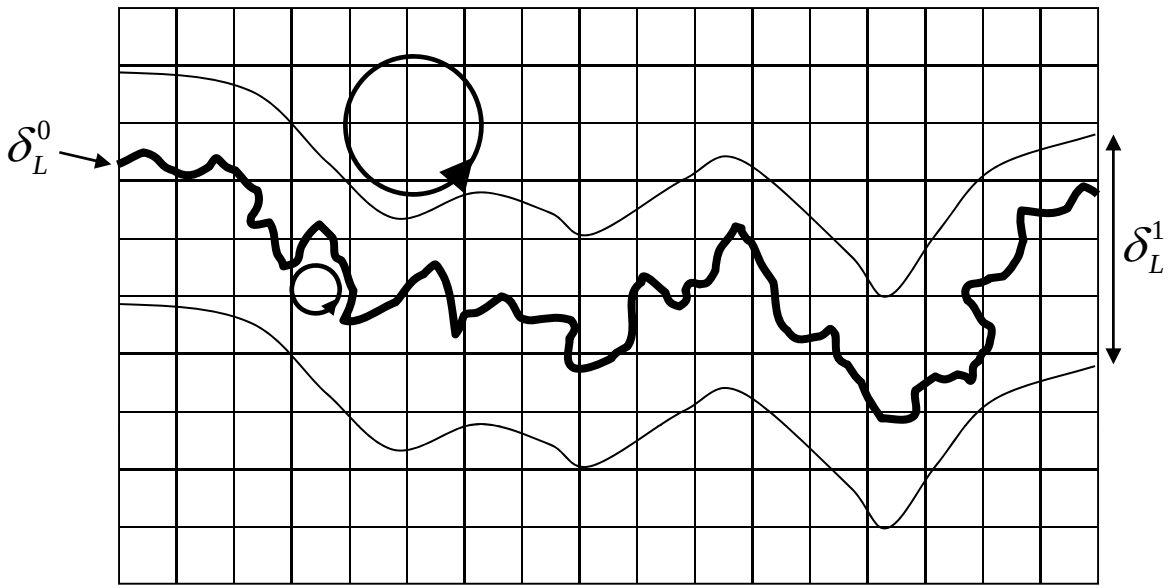


Mean axial velocity



- **Central and corner recirculation zones present.**

Thickened Flame Model



Local thickening based on gradients of H_2O and RR

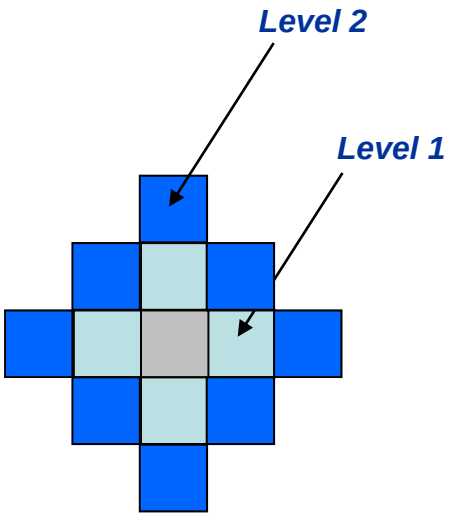
$$s_L^0 \propto \sqrt{D \cdot RR}, \qquad \delta_L^0 \propto \frac{D}{s_L^0} \qquad D_a = \frac{\tau_t}{\tau_c} = \frac{l_t s_L^0}{u' \delta_L^0}$$

- **Increase *D* and reduce *RR* by factor "*F*".**
  - Flame propagates at same laminar flame speed.
- **Decrease in Da# decreases flame response to turbulent scales. Must model this effect with a sub-filter efficiency function "*E*".**

Calculation of $u'_{\Delta e}$

- **Method 1: Velocity Operator (Colin et al.)**
  - Requires 3rd derivative of velocity field.
  - Large degree of numerical error.

$$u'_{\Delta_e} = 2\Delta_x^3 \nabla^2 \left(\nabla \times \bar{u} \right)$$



- **Method 2: Direct Filtering**
  - Recursively filter the velocity field "n" times.
  - n=4 for filter width of 5 cells (linear).
    - Averages over 125 cells for 3D hexahedral mesh

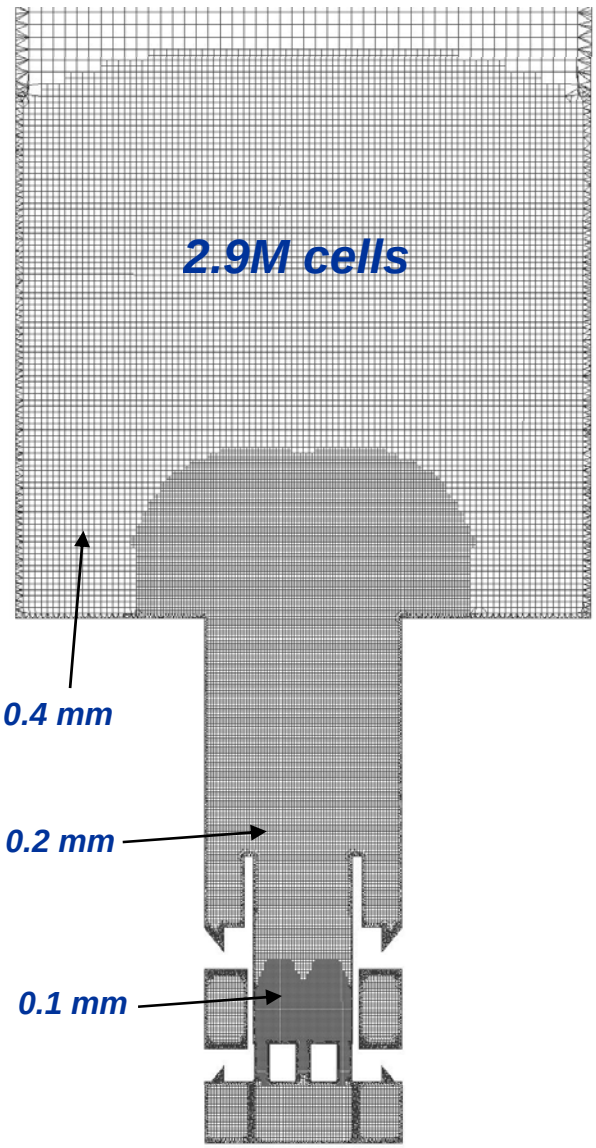
$$u'_{\Delta_e} = \left[\left(u_x - \tilde{u}_x \right)^2 + \left(u_y - \tilde{u}_y \right)^2 + \left(u_z - \tilde{u}_z \right)^2 \right]^{1/2}$$

LES Approach (FLUENT)

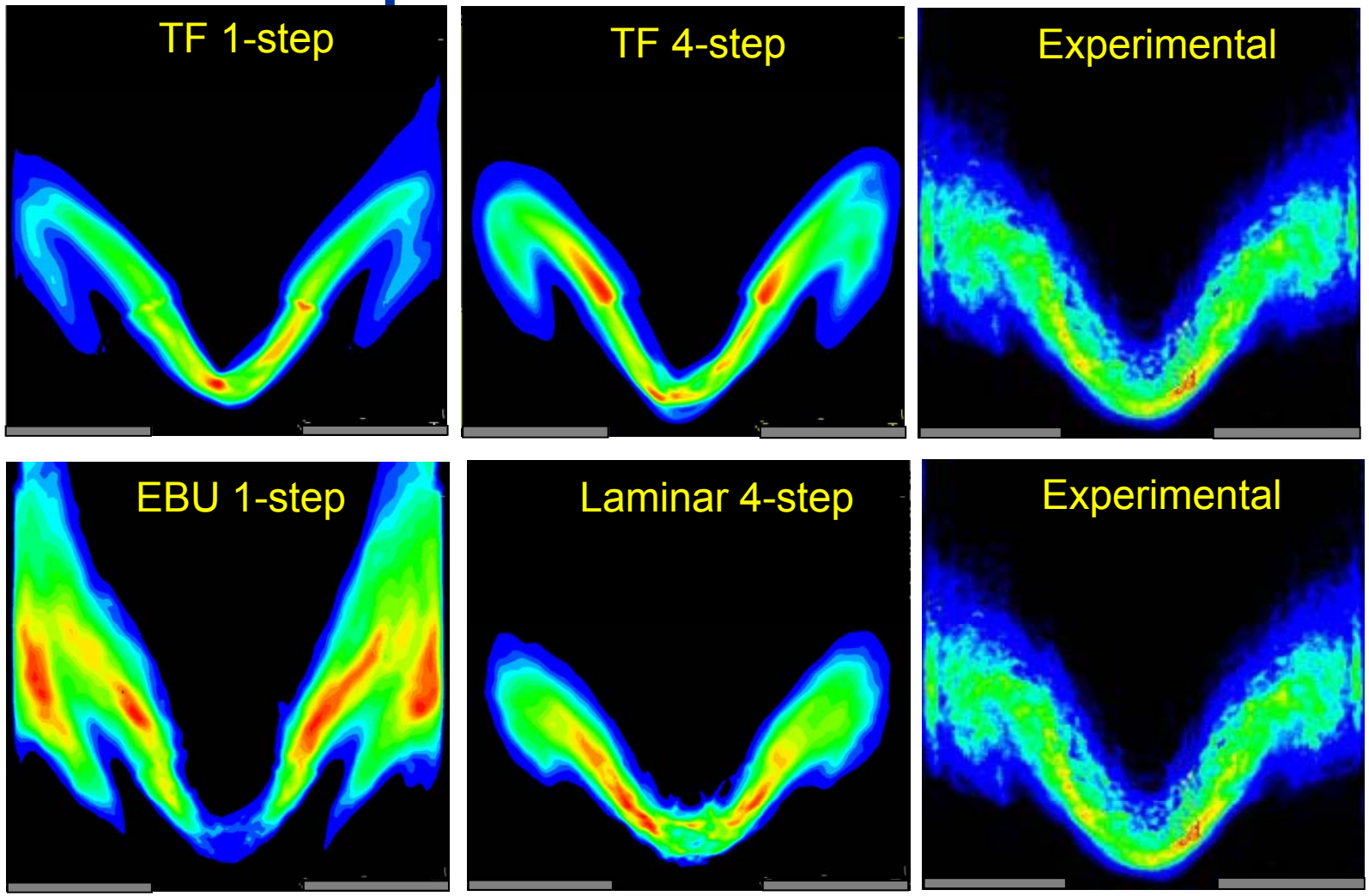
- **Grid through swirler**
  - Wall upstream to specify flow-split (18.2%).
- **LDKM sub-grid viscosity.**
- **BCD for momentum.**
- **2nd Upwind for scalars**
- **Inside wall temp from RANS.**
- **4 simulations:**
  - 1-step: TF and EBU
  - 4-step: TF and Laminar

$$CH_4 + 2H + H_2O \rightarrow CO + 4H_2$$
$$CO + H_2O = CO_2 + H_2$$
$$2H + M \rightarrow H_2 + M$$
$$O_2 + 3H_2 = 2H + 2H_2O$$

$$[OH] = [H][H_2O]/([H_2]K_3)$$

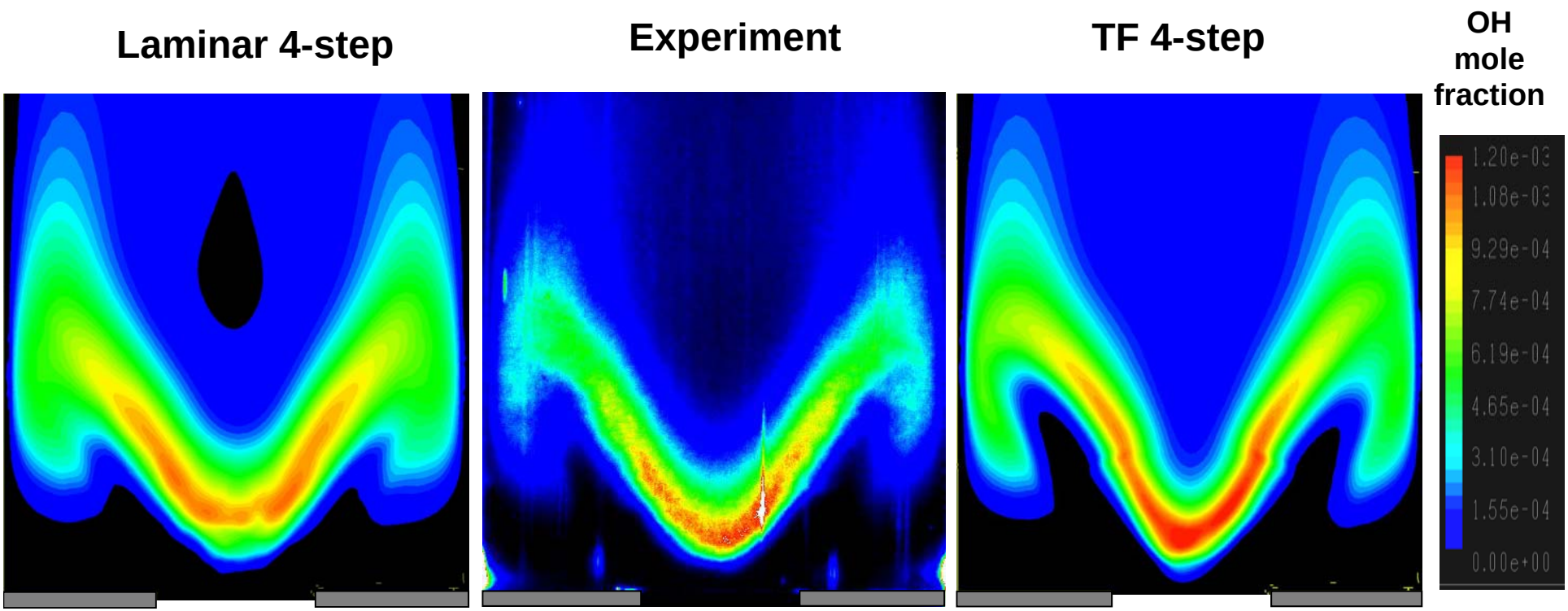


Comparison of Heat Release



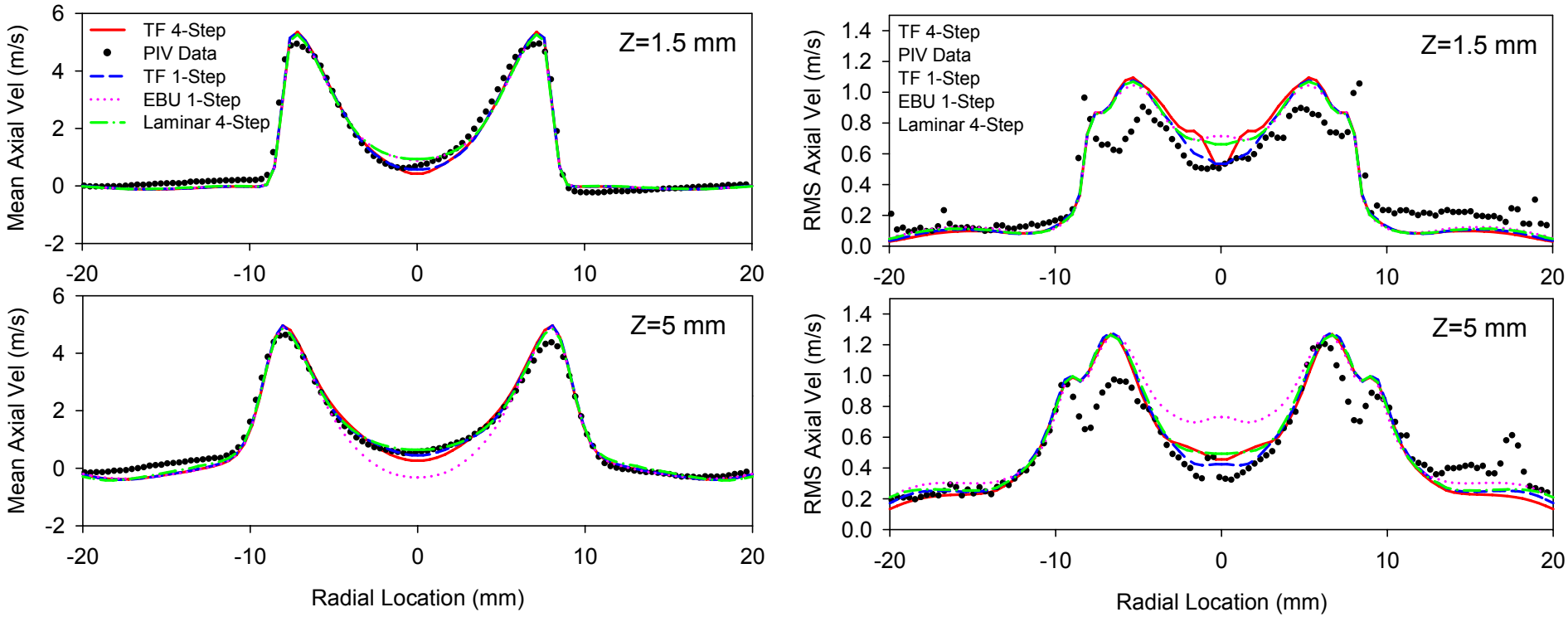
- **Both 1-step and ARM4 predict similar profiles. ($u'/S_L \sim 5$)**
- **Some error in experimental data due to noise in areas of low OH concentration (near the walls).**

Comparison with OH concentration



- **LES with ARM4 chemistry does a good job of predicting flame shape. Does tend to over-predict OH near walls and in post-flame zone.**

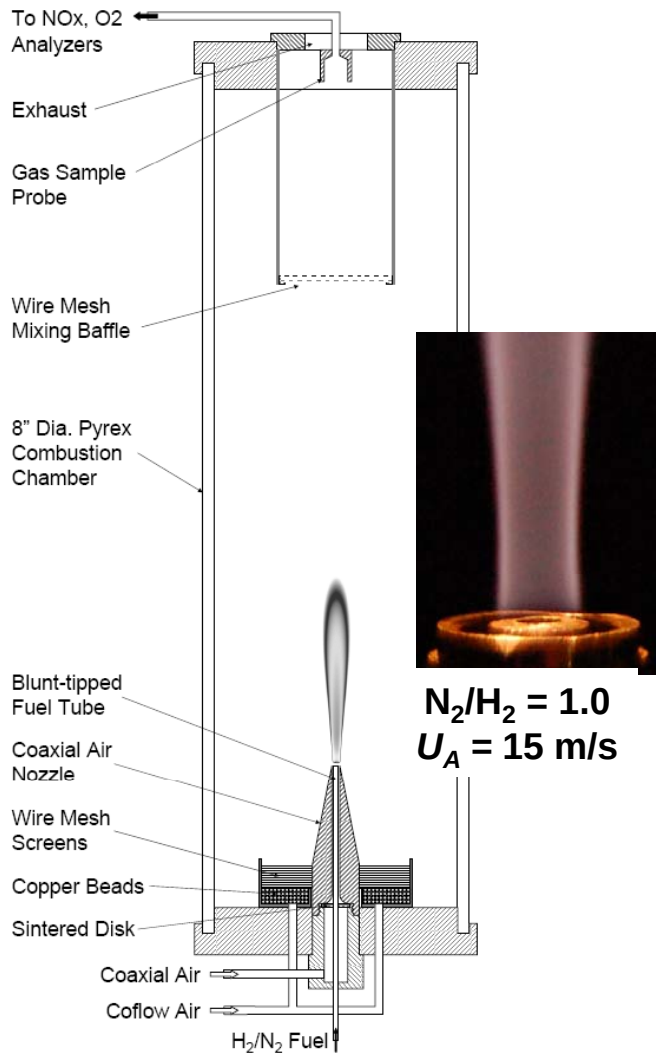
PIV LES Comparison (CH_4/Air ϕ=0.7)



- **TF model works well for the case studied here.**
  - Low levels of u', good grid resolution and modest thickening factors.
- **Next step is to apply the model to larger scale combustors and higher velocities (higher Re_T).**
- **Preferential diffusion effects for H_2 fuels needs to be accounted for.**

Hydrogen Dilute Diffusion Flame Studies

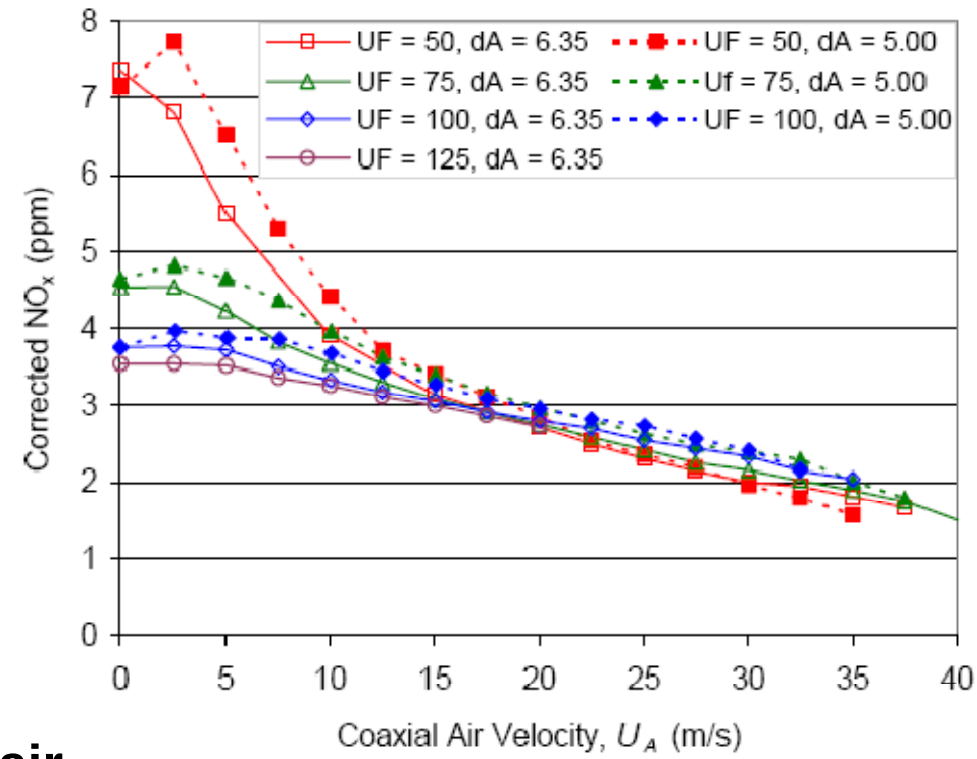
- **Jet diameter: d_F = 1.45 mm**
- **High-velocity coaxial air diameters: d_A = 5.00 & 6.35 mm**
- **Nitrogen dilution of hydrogen or coaxial air streams**
- **Low velocity coflow air supplied at less than 0.25% of the jet exit velocity**
- **Wire mesh mixing baffle used to eliminate NO_x profile at exhaust**
- **NO_x measurements corrected using measured O_2 content in dry exhaust gas and known dilution level**
  - Equivalent to Emission Index (g NO/kg H_2)



N_2/H_2 = 1.0
U_A = 15 m/s

Atmospheric Pressure NO_x Measurements

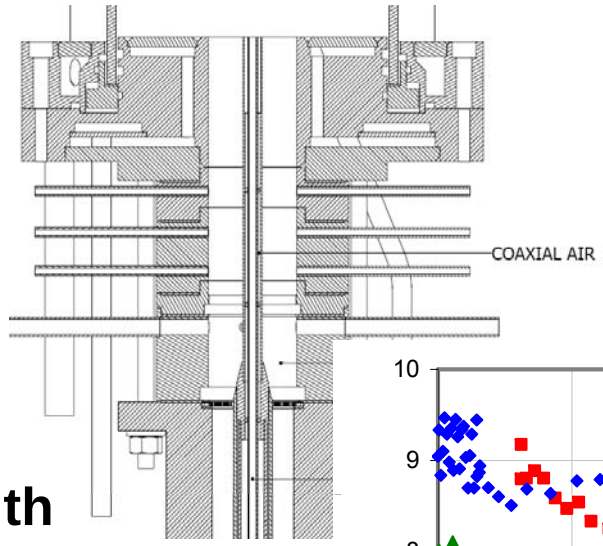
- **NO_x measurements taken in absence of recirculation effects**
- **All measurements taken with 50/50 H_2/N_2 fuel**
- **NO_x generally decreases with u_a, as expected**
  - Reduced flame volume
  - Reduced flame residence time
- **NO_x emissions at least halved with use of high-velocity coaxial air**



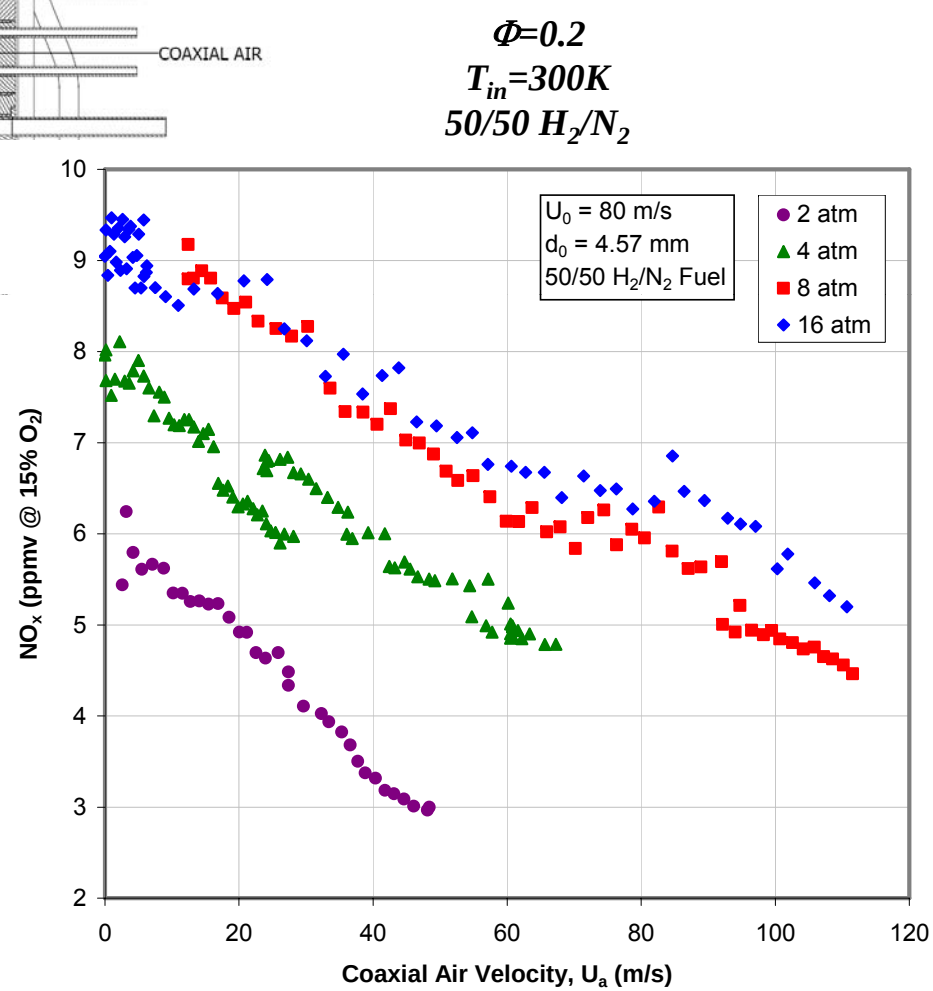
- **Global flame strain for coaxial air flames is not an appropriate Damköhler number mixing time scale:** $1/t_{mix} \neq (u_0 - u_a)/d_0$
- **Mixing time reduced with addition of coaxial air**

$$\frac{EINO_x}{V_f/u_0 d_0^2} \propto \left(\frac{u_0}{d_0}\frac{d_0^*}{L_f}\right)^{1/2} \propto \left(\frac{u_0}{d_0} f_s\left[1 + J_a/J_0\right]^{1/2}\right)^{1/2}$$

High Pressure Coaxial Air NO_x Emissions

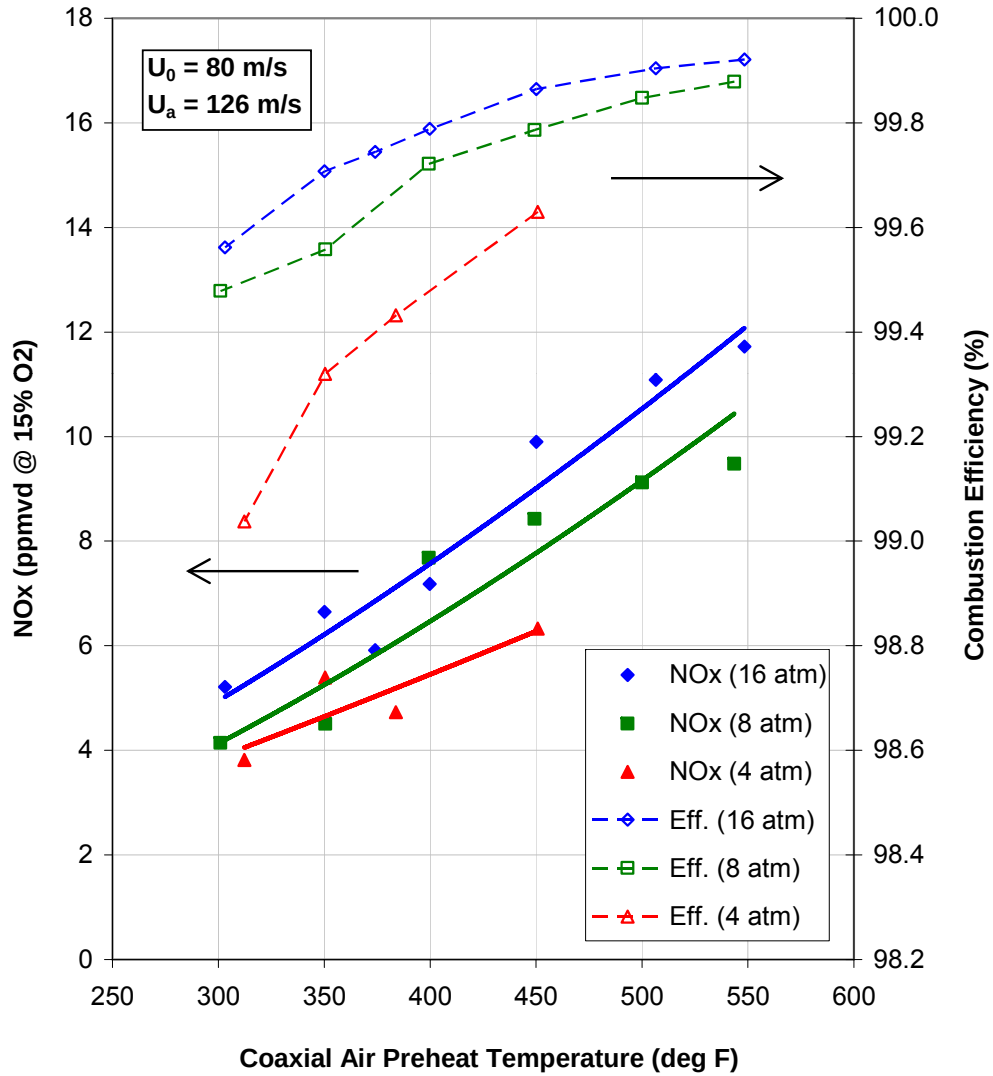


- **NO_x decreases with increasing coaxial air velocity**
- **NOx increases with pressure**
  - Increase in reaction rates relative to mixing
- **Higher coaxial air velocities attained**
  - Increase in flame stability with pressure
- **At 16 atm, low of 5.2 ppm NO_x @ 15% O_2**



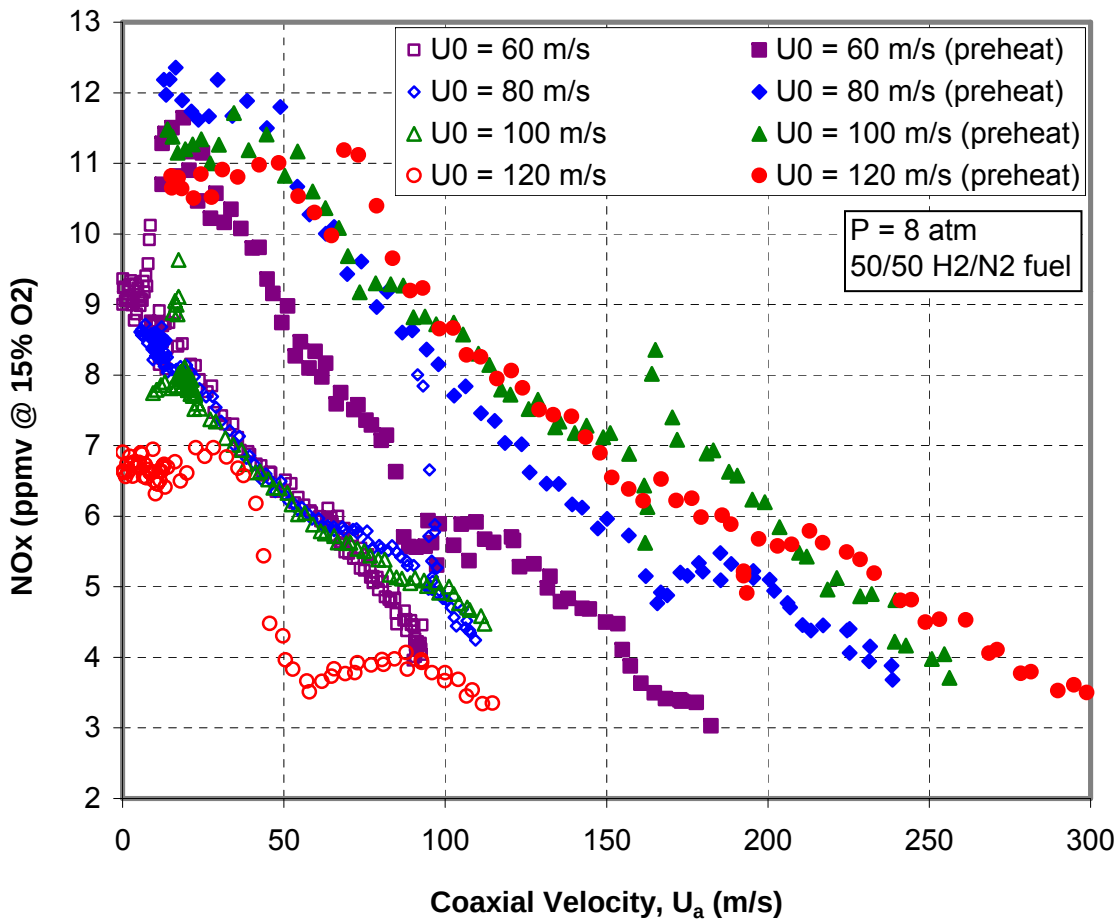
Effect of Air Preheat at Constant Velocity

- Data taken for various coaxial air preheat temperatures, at constant fuel and air velocities
- NO_x increases with pressure and preheat temperature
- Combustion efficiency and flame stability also both increase with pressure and preheat temperature



Effect of Air Preheat on NO_x at 8 atm

- Coaxial air preheated from ~350 K to ~550 K as coaxial air velocity increased
- Air preheating increases NOx
- Coaxial air stability limits significantly increased
- Lowest attainable NOx may be reduced with coaxial air preheat



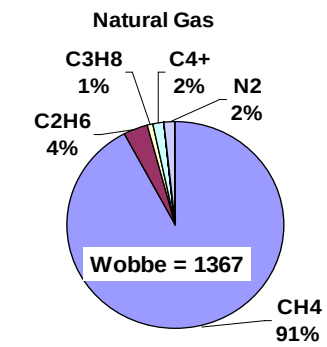
Why is Fuel Flexibility Important for the Future of Combustion Applications?

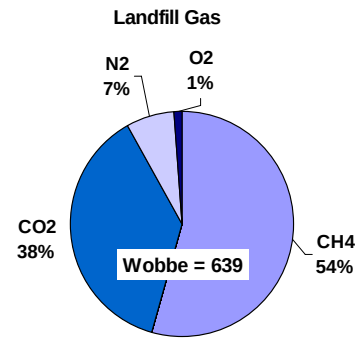
- **Economics**
  - Rising cost of natural gas
  - Efficiency improvements result in savings.
  - Alternatives becoming more economical
  - Carbon trading?
- **Supply**
  - How long will it last?
  - Reduces our dependence on foreign fuel supplies
- **Environment**
  - Reduces greenhouse gas and other emissions
    - Utilizing waste and flare gases
    - Carbon capture/removal

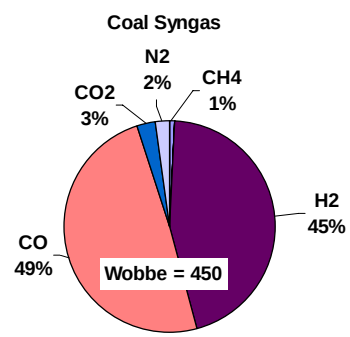
Focus of Fuel Flexibility Efforts

- **Began as an EERE program to look at fundamental effects of fuel composition on flame characteristics.**
  - Interest in bio-fuels
- **Now a more encompassing effort to examine fuel composition effects on combustion.**
  - Low BTU fuels
    - Effects of CO2 dilution on combustion properties.
    - Combustion dynamics issues.
  - LNG and assessment of indices like Wobbe number.
    - Importing NG in the form of liquified natural gas (LNG) is expected to increase by almost 35% by 2010
  - Model validation under wide range of fuel compositions.
    - Can I predict how my NG combustor will operate with digester gas?
  - High-hydrogen fuels (syngas, pure H_2).
  - CO_2 recycle for carbon capture.
  - Sensors.

Carbon management is an overarching issue for all combustion applications!



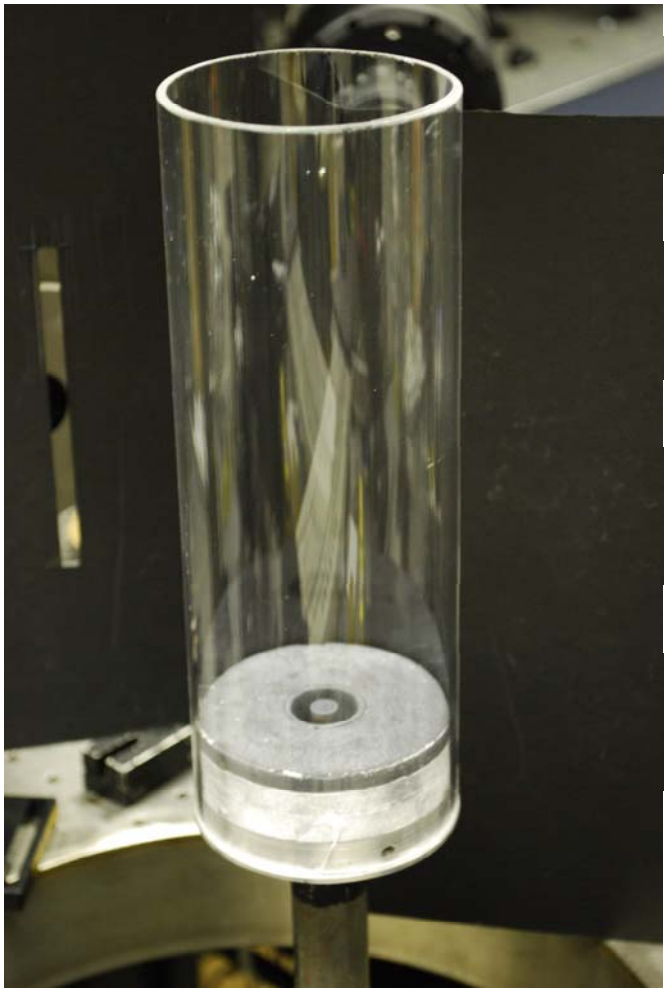




Lab-Scale Burner for Fuel Flex Studies

D_{comb}= 80 mm
D_{inlet}= 22 mm
L_{comb}= 200 mm

Designed for fuel-flex studies

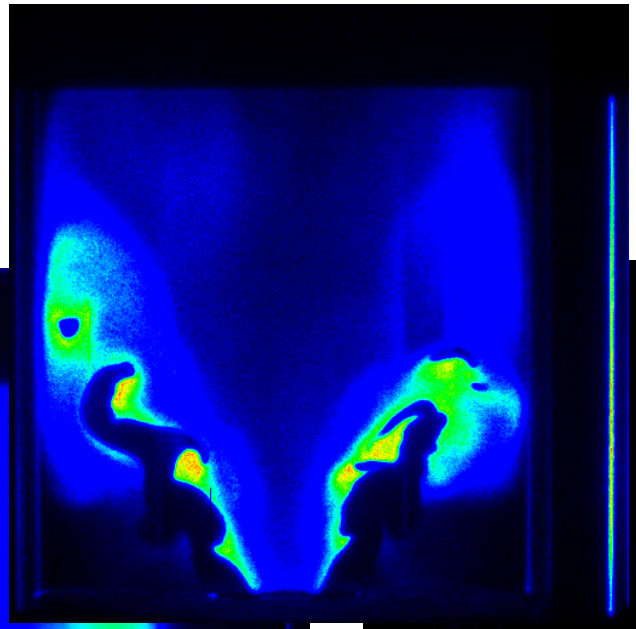


100 slpm air
CH_4 Φ=0.8
~ 4 kW

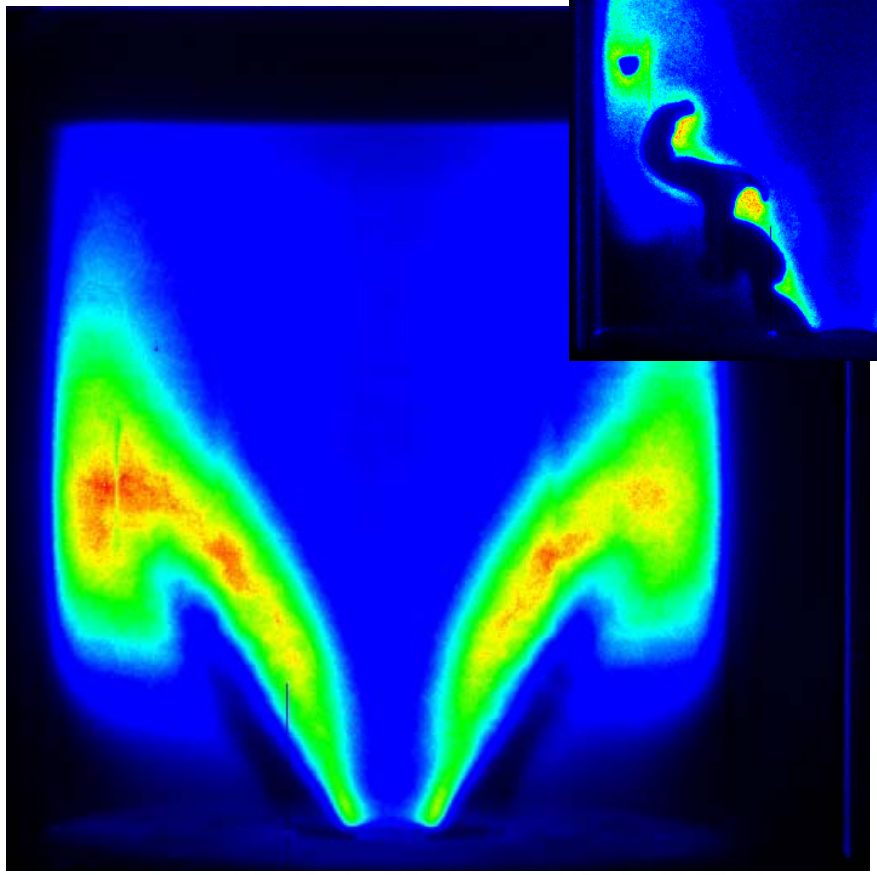
OH-PLIF Characterization

200 mm long combustor
100 slpm air
CH_4 Φ=0.8

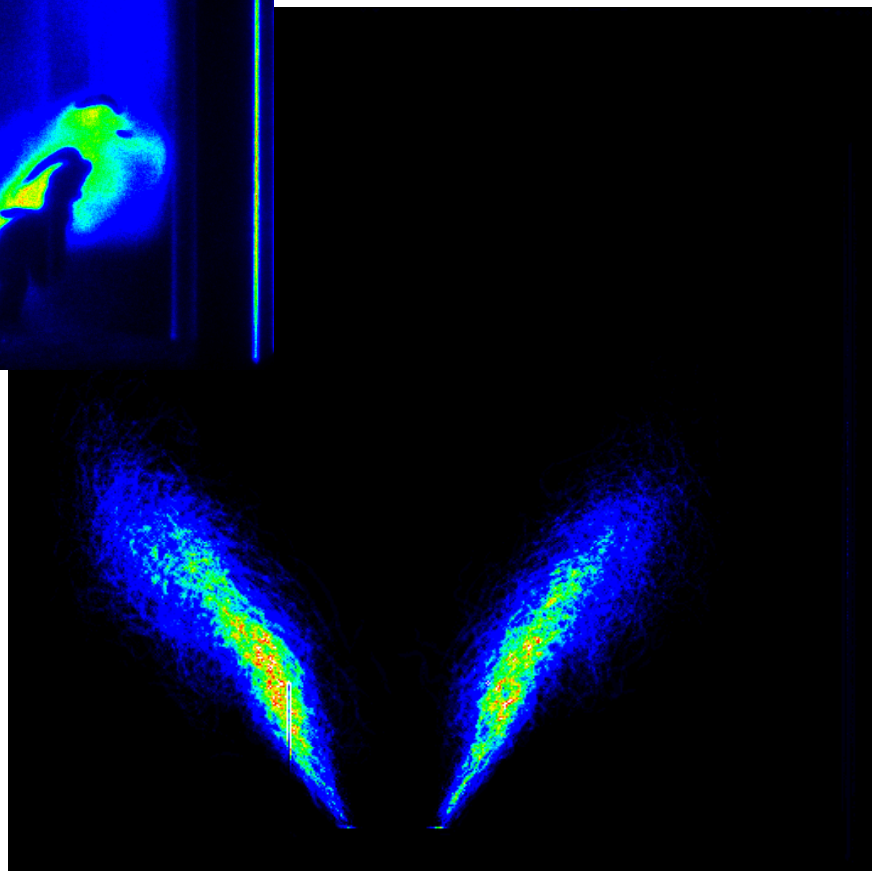
Instantaneous OH



Mean OH

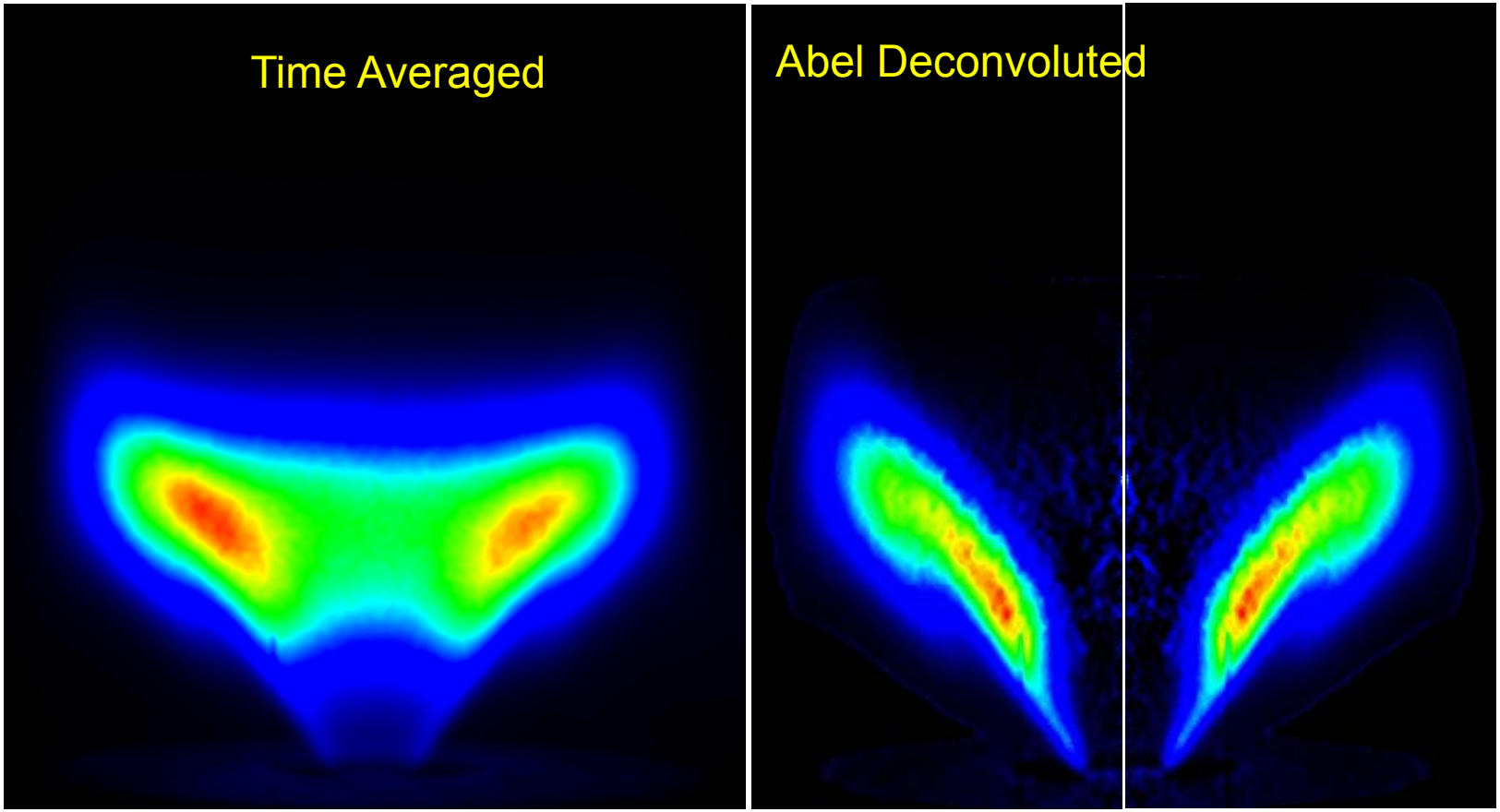


Flame-front probability



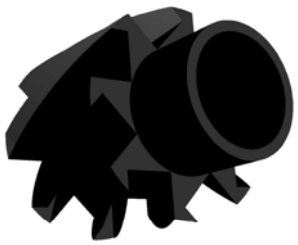
Chemiluminescence

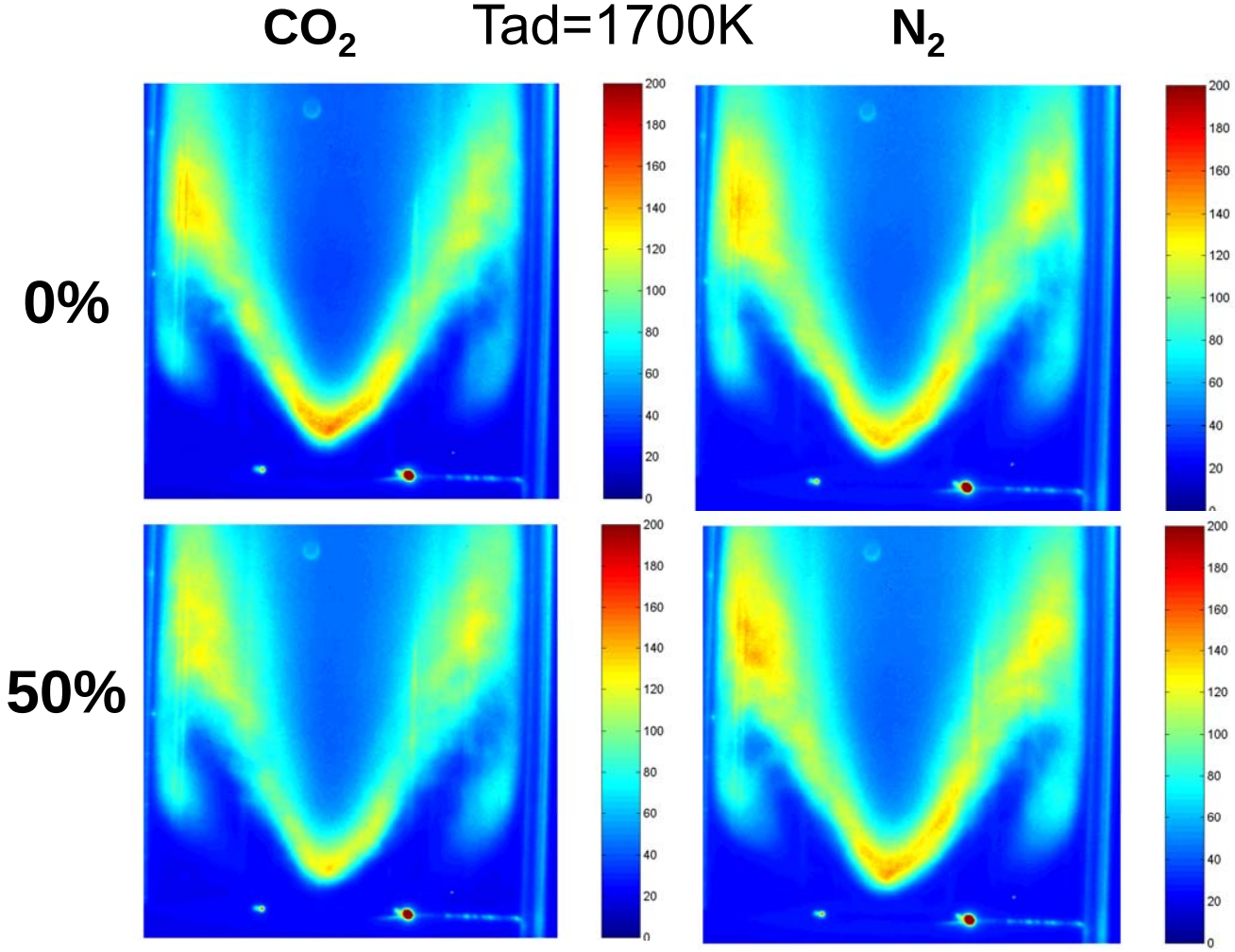
200 mm long combustor
100 slpm air
CH_4 Φ=0.8



Next step is to vary fuel composition

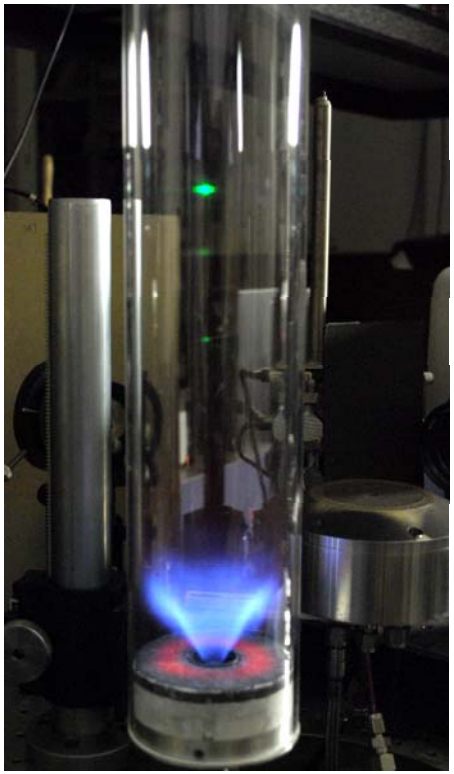
Effect of CO_2 Dilution of Flame Shape

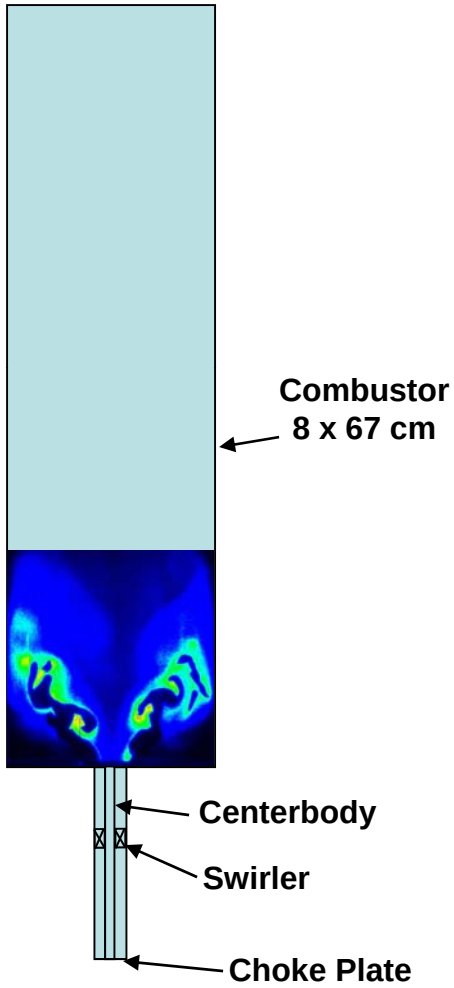




- **Slight increase in flame brush length with CO_2 addition. No effect of N_2 addition. Radiation?**

Combustion Instability in a Lab-Scale Swirl Stabilized Combustor





Experimental Conditions

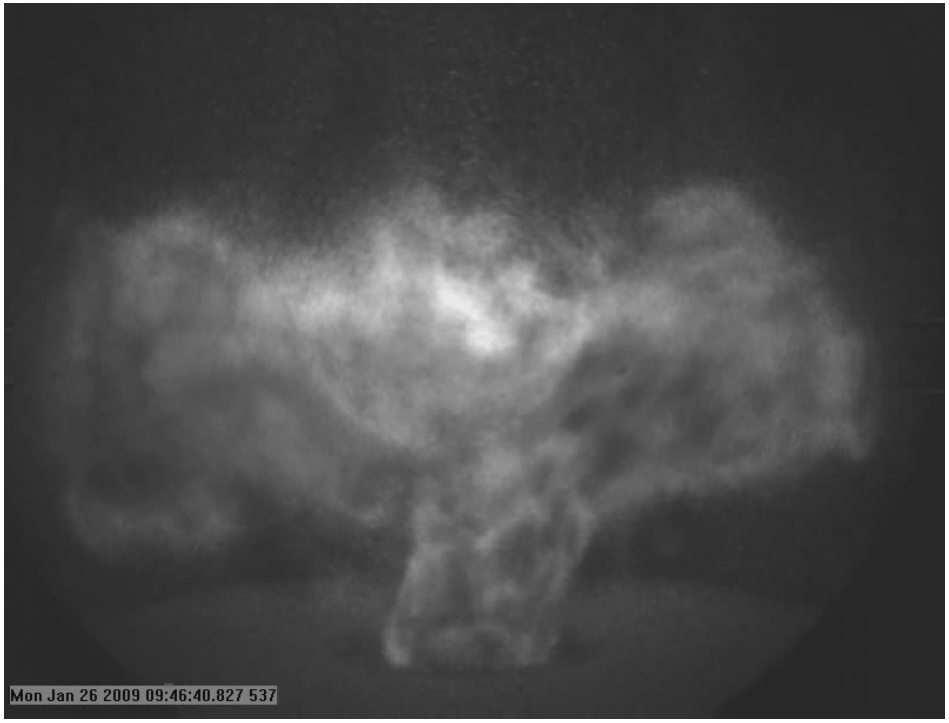
- 109 slpm Air-CH_4
- ϕ = 0.80
- 8 m/s inlet velocity
- 160 Hz longitudinal instability driven by vortex shedding

LES Modeling

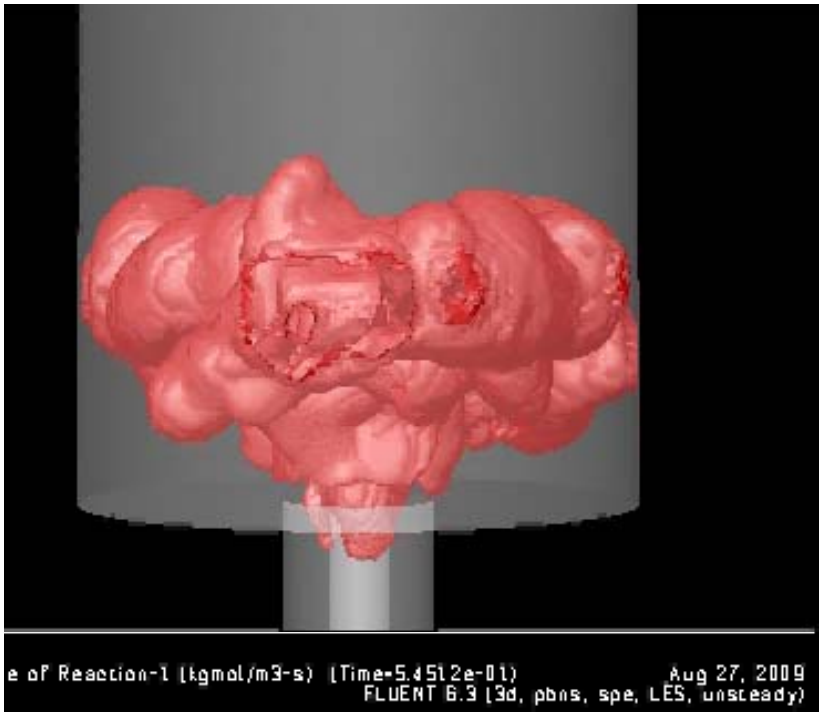
- FLUENT
- 1.5M cells
- Thickened Flame Model
- 1-step CH_4/Air
- Dynamic Smagorinsky
- Domain: from choke plate through combustor exit (large damper to simulate room)

LES of Combustion Instability

High Speed Imaging of Chemiluminescence (4000 fps)

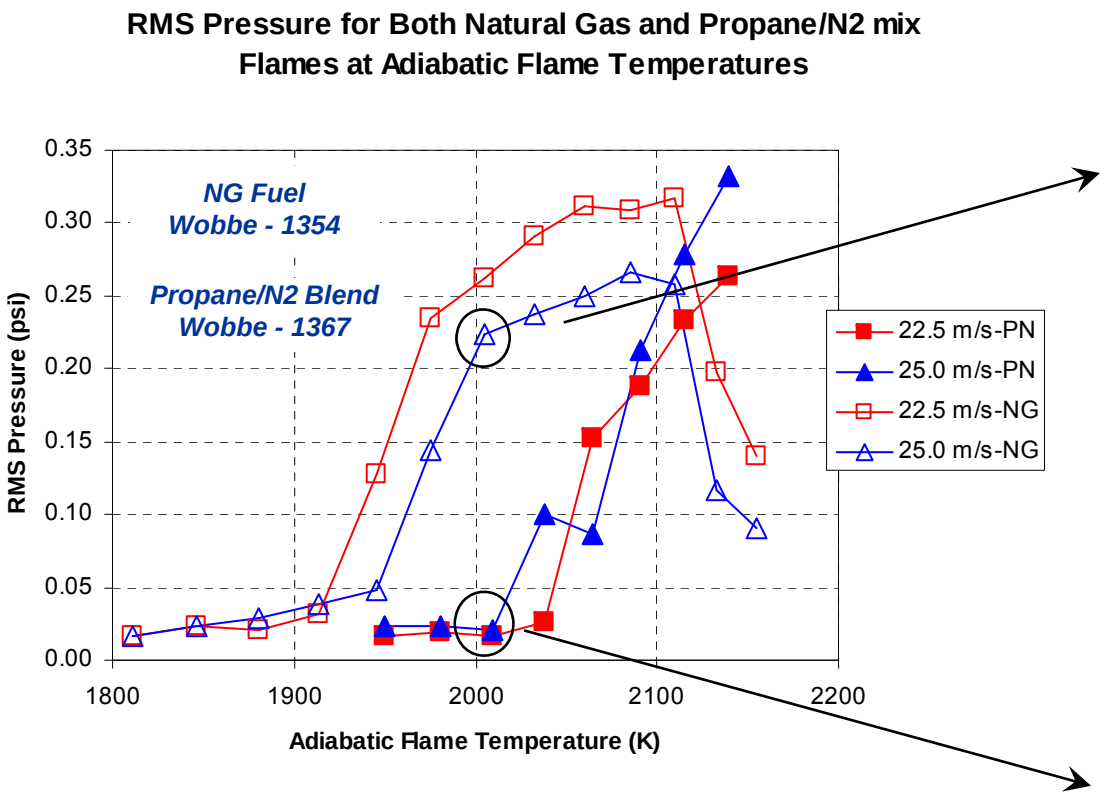


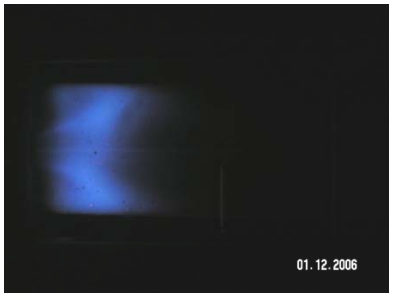
Iso-surface of reaction rate

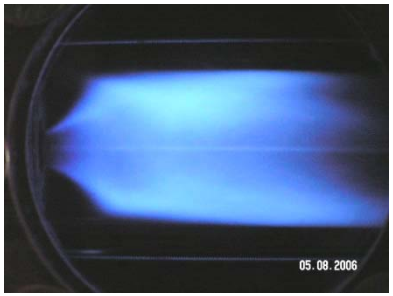


- **LES captures 160 Hz instability (both pressure and heat release).**
- **Flame response qualitatively similar.**

Variations in Dynamic Response Due to Fuel Variability - Physical or Chemical?

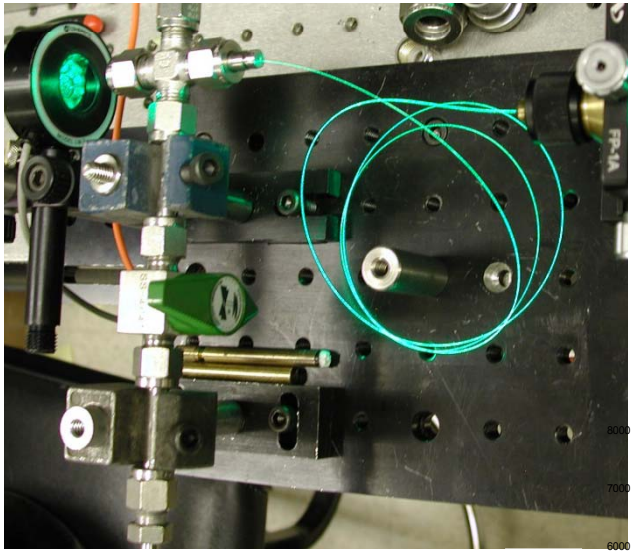


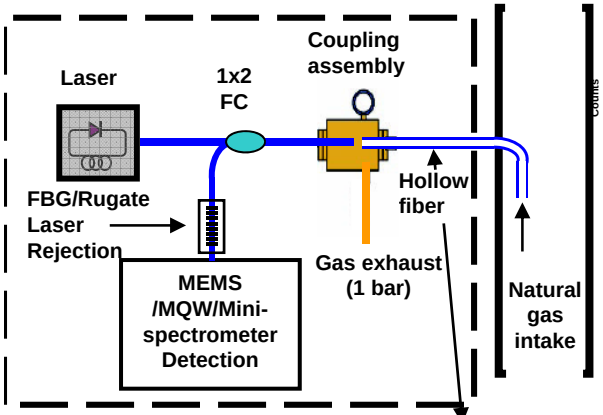


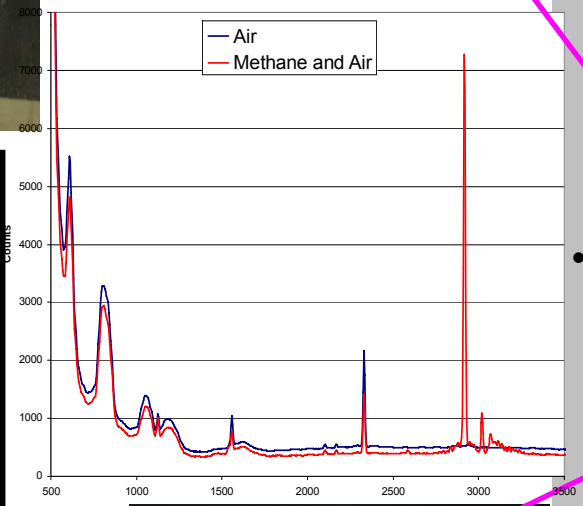


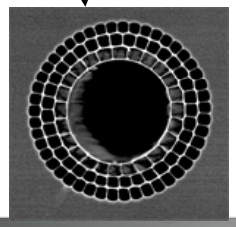
- ***Are changes in the dynamic response the result of physical (mixing and acoustics) differences or chemical?***

RAMAN Spectroscopy Sensor Development



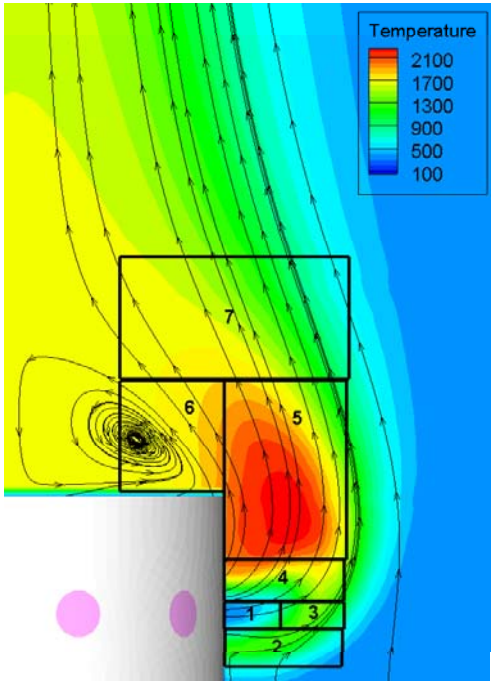


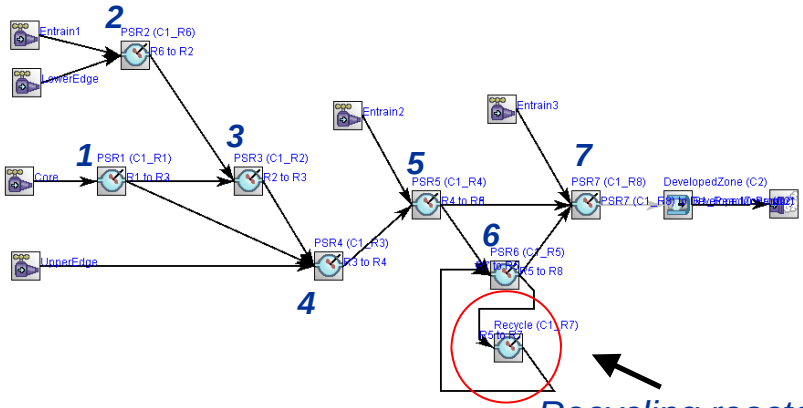




- **Purpose/Goal**
  - Detect natural gas species concentration changes in real time for improved burner control
- **Accomplishments**
  - Advanced Fiber Optics tested in Raman Gas Composition Sensor System
    - Hollow Core Photonic Bandgap Fiber
    - Ag Coated Capillary
  - Successful measurements of Raman scattering of multiple gas species
    - Sensitivity improved with new Ocean Optics spectrometer
- **Other Progress**
  - 30 milliwatt Nd:Vanadate Laser
  - Applied Optics paper submitted
  - LACSEA Poster presented
  - CLEO Poster presented

Utilize CFD Results for input to PSR's





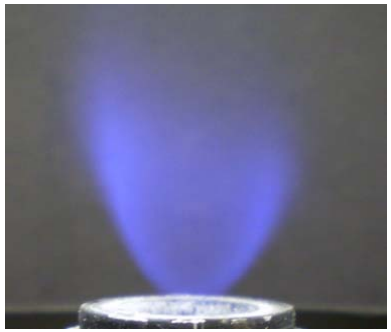
Recycling reacted products

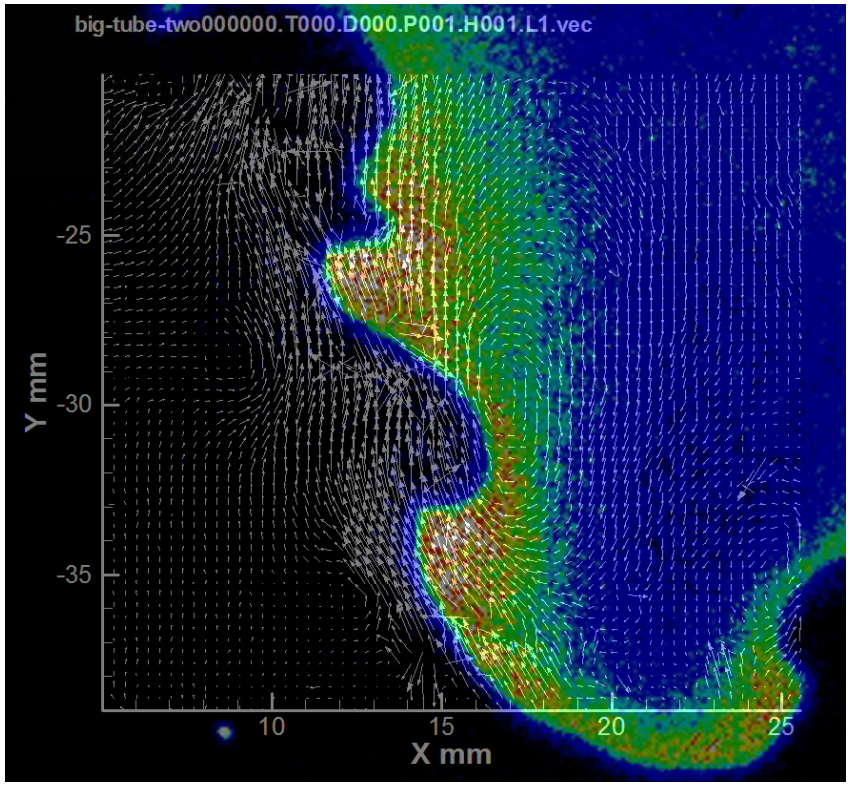
- **Utilize skeletal mechanism in CFD or non-reacting flows**
- **Divide flow field into collection of reactor networks**
- **Integrate regions to determine**
  - Mass flow or velocity
  - Residence times
  - Temperatures
- **Utilize detailed chemical mechanisms in reactor model**

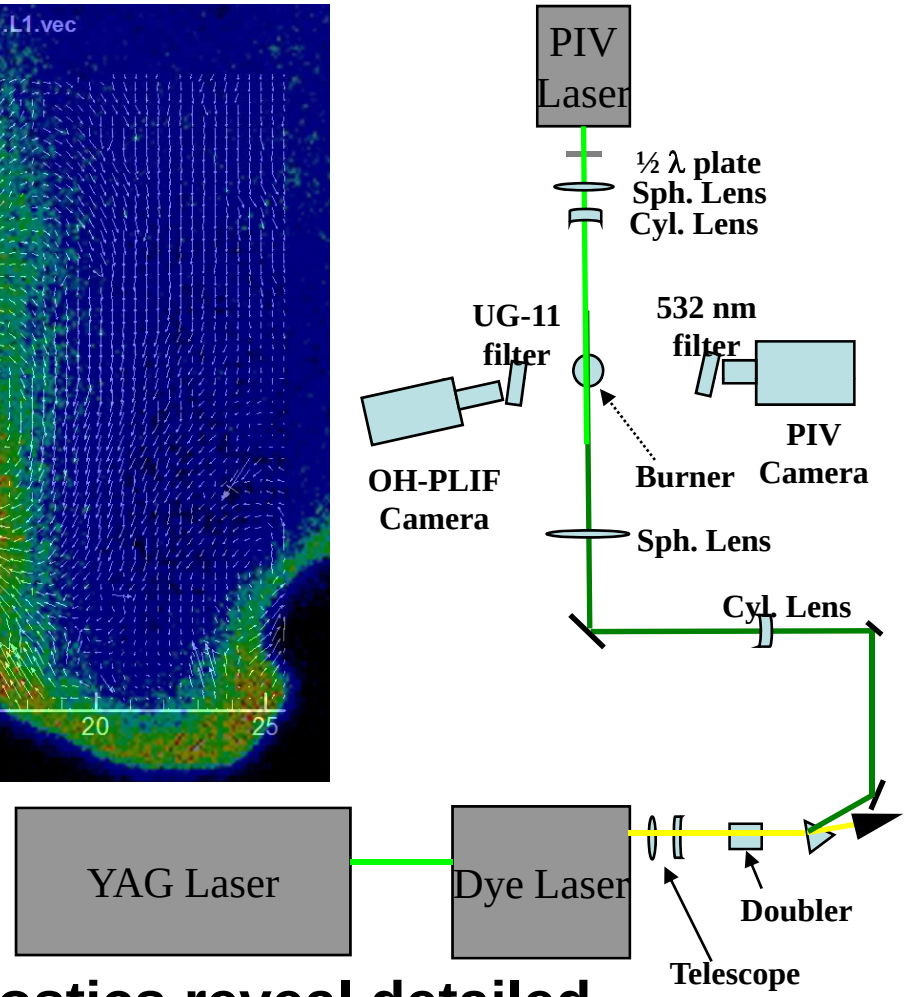
Combustion Diagnostics Development

Simultaneous OH-PLIF and PIV

LSI, CH4/Air,
ϕ=0.62



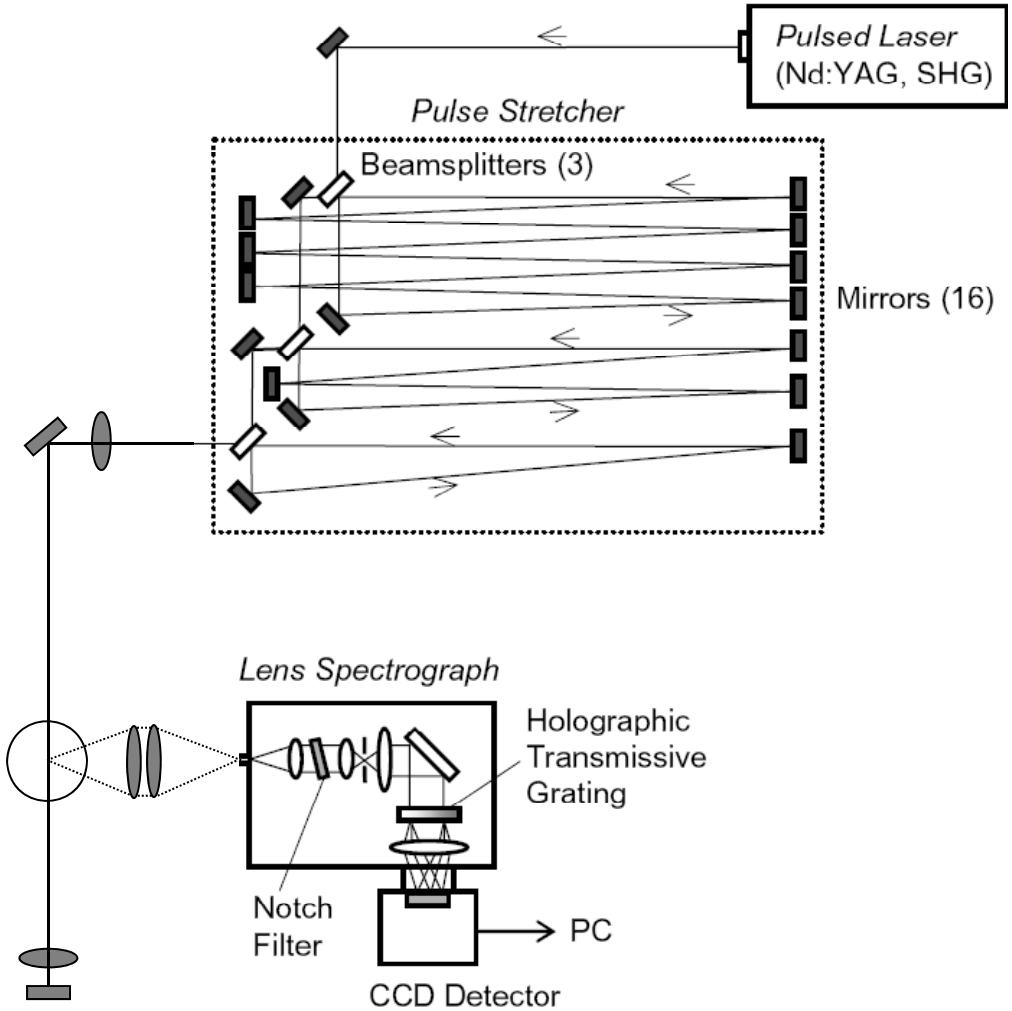




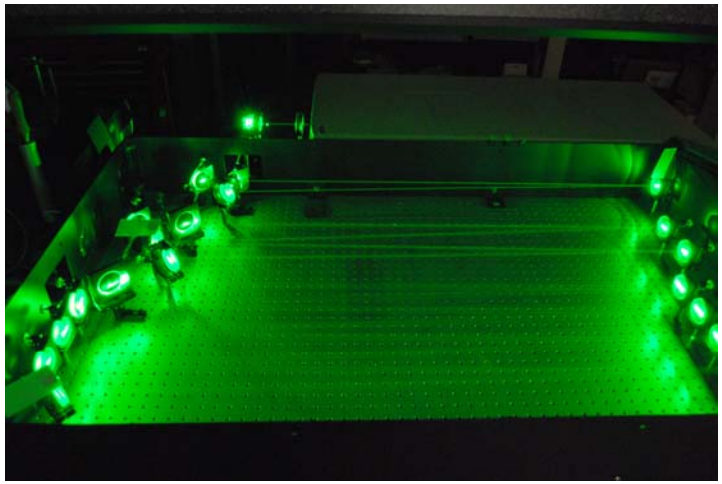
- **Simultaneous planar diagnostics reveal detailed information on flame structure.**

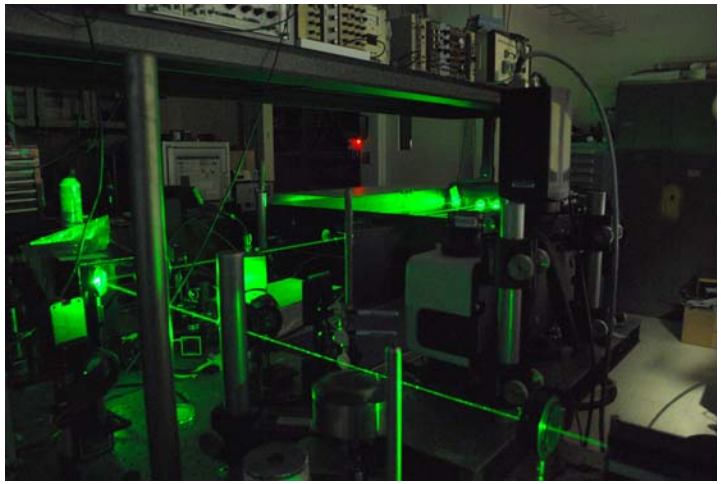
Spontaneous Raman Scattering (SRS)

1 Joule at 532 nm, PIXIS 2048 and PI-MAX 1024
1-D line imaging (16 mm)
T, N2, O2, CO2, H2O, CH4, CO, H2



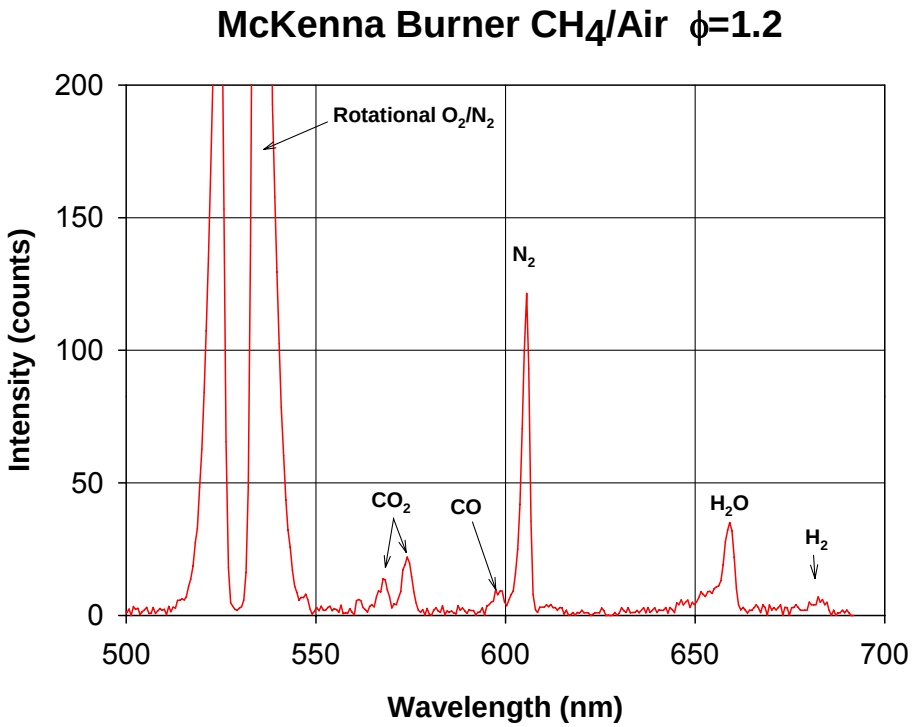
Pulse stretcher



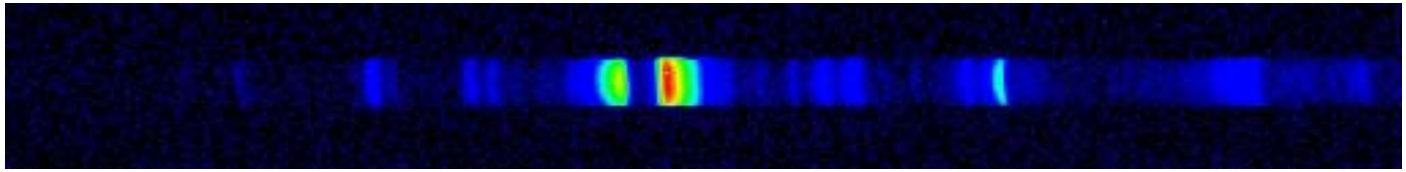


Status of SRS System

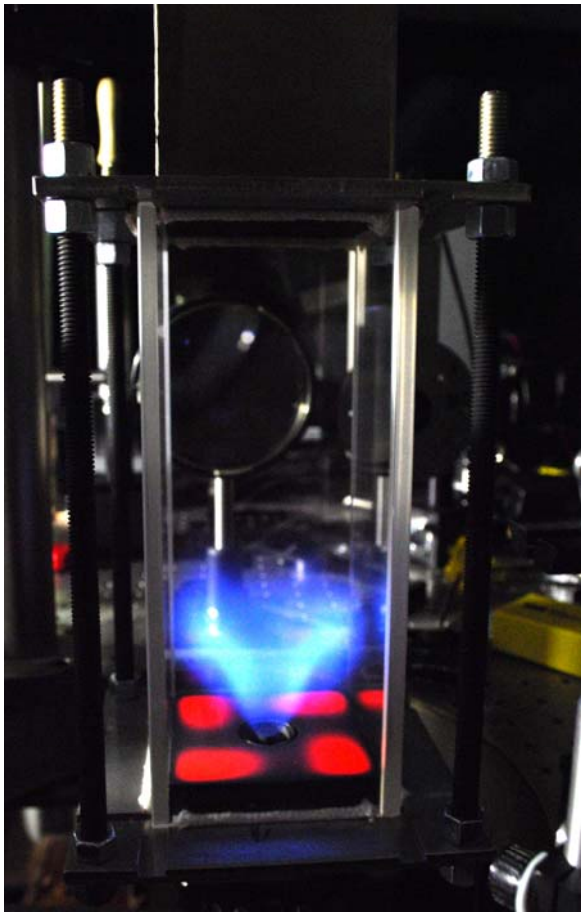
- **Optimizing collection optics and camera configuration.**
- **Developing data reduction routine to account for cross-talk.**
- **Developing calibration procedure using McKenna burner and heated gases.**
- **Application in swirl-stabilized burner (square chamber) to complement PIV and OH-PLIF data.**



Raman spectra (100 shot avg.) from a rich methane-air flame (ϕ=1.2) at 6 mm from the burner face. Vibrational transitions for all major species are identified.



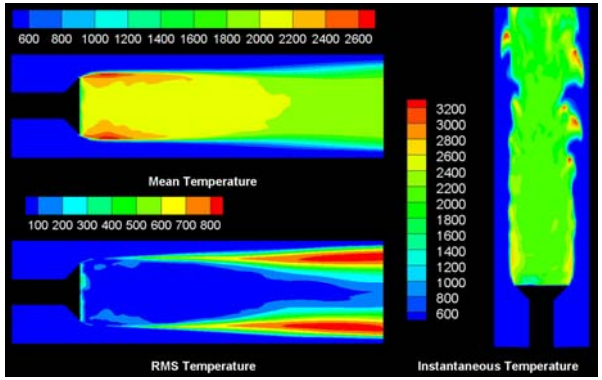
Getting Away from the “Round” Combustor



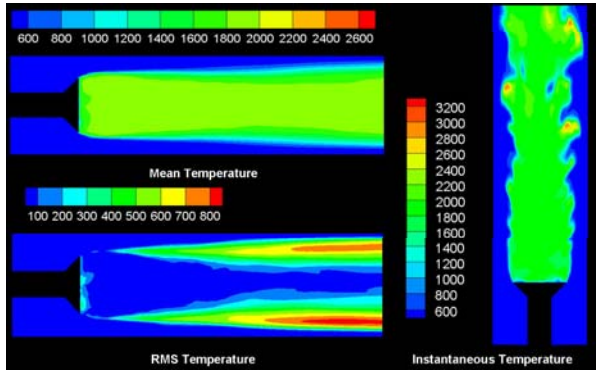
- **Optical quality quartz windows reduce problems with reflections, beam steering and image distortion.**
- **For LES validation chamber shape is not an issue.**

Modeling Combustion Emissions Using LES: An Assessment of SGS Turbulent Combustion Models

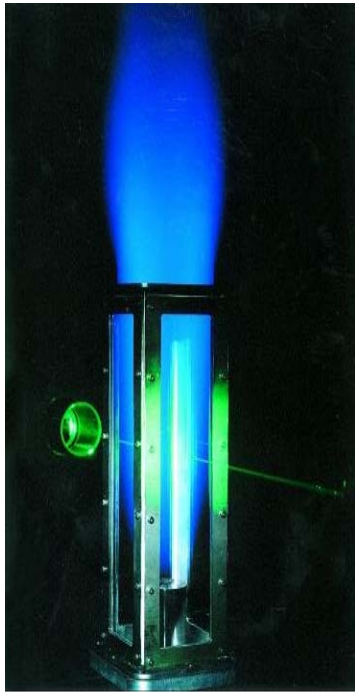
Eddy Dissipation Model



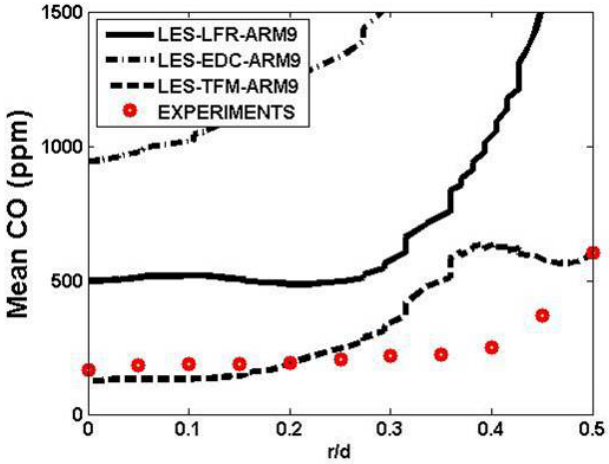
TF Model



Vanderbilt Bluff-Body Combustor

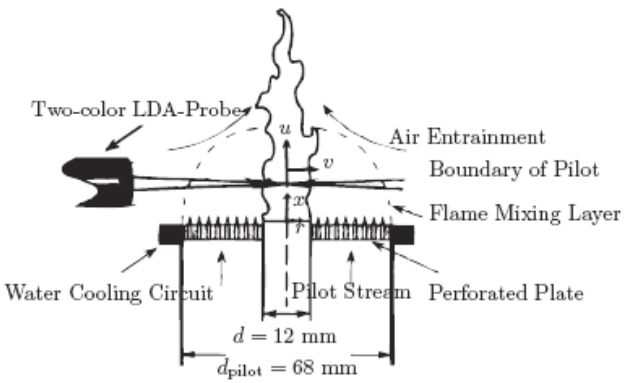


Mean CO, x/d=0.6



- **Project to assess capability of various SGS combustion models to predict emissions using the FLUENT code.**

Filtered Density Function for LES of Lean Premixed Methane Flames



Turbulent Bunsen flame experiment from Chen.

5-step, 9-species ARM

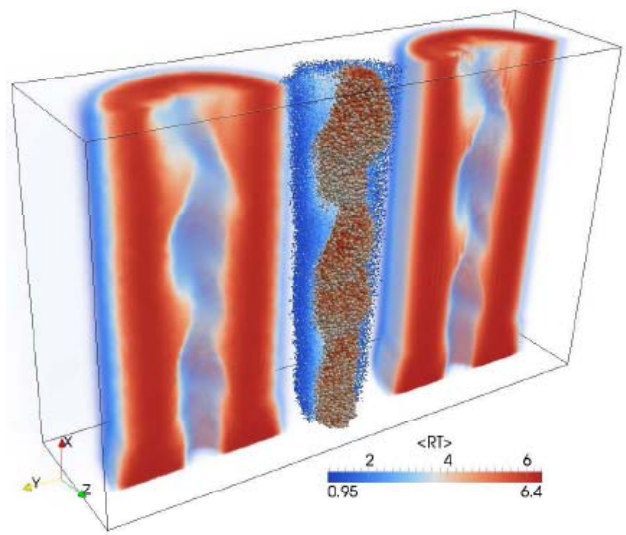
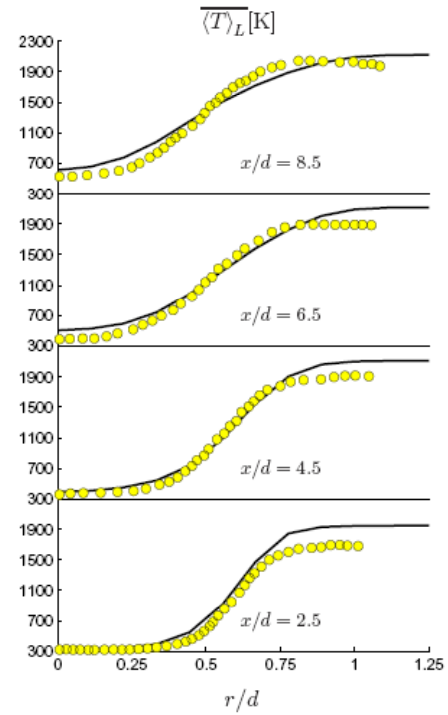


Figure 5: The instantaneous fields as obtained from MC (left), FD (right), and the particle field (mi

Mean temperature profiles, lines=LES, symbols=experiment



- **Project to assess capability of LES/FDF methods for lean premixed flames. Looking at emissions, flame stability, etc.**

University Coal Research Programs

Stanford University – "Enabling Advanced Modeling and Simulations for Fuel-Flexible Combustors" (Heinz Pitsch)

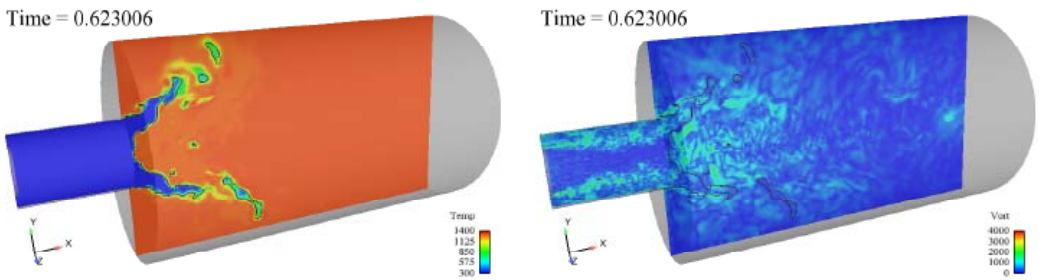


Figure 3: Instantaneous profiles of temperature (left) and vorticity (right) for the simulation of the lean hydrogen premixed low-swirl injector.

LBNL Low Swirl Injector, H_2/Air, ϕ=0.35

Virginia Tech – "Experimental and Computational Investigations of Boundary Condition Effects on CFD Simulations of Thermo-Acoustic Instabilities" (Bob West)

- The goal of the proposed work is to determine the sensitivity of transient thermo-acoustic Computational Fluid Dynamics (CFD) simulations to poorly defined, or misrepresentation of prescribed acoustic boundary conditions.