# Quantitative Thermochemical Measurements in High-Pressure Gaseous Combustion

Jun J. Kojima (presentor)
Ohio Aerospace Institute, 22800 Cedar Point Rd, Cleveland, OH 44142, USA

David G. Fischer
NASA Glenn Research Center, 21000 Brookpark Rd, Cleveland, OH 44135, USA

## Abstract

We present our strategic experiment and thermochemical analyses on combustion flow using a subframe burst gating (SBG) Raman spectroscopy. This unconventional laser diagnostic technique has promising ability to enhance accuracy of the quantitative scalar measurements in a point-wise single-shot fashion. In the presentation, we briefly describe an experimental methodology that generates transferable calibration standard for the routine implementation of the diagnostics in hydrocarbon flames. The diagnostic technology was applied to simultaneous measurements of temperature and chemical species in a swirl-stabilized turbulent flame with gaseous methane fuel at elevated pressure (17 atm). Statistical analyses of the space-/time-resolved thermochemical data provide insights into the nature of the mixing process and it impact on the subsequent combustion process in the model combustor.

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# Quantitative Thermochemical Measurements in High-Pressure Gaseous Combustion


DR. JUN KOJIMA*
*Combustion Scientist*
RTB/OAI

DR. DAVID FISCHER
*Optical Scientist*
RTB


JULY 12-13, 2012 @ GE GLOBAL RESEARCH CENTER

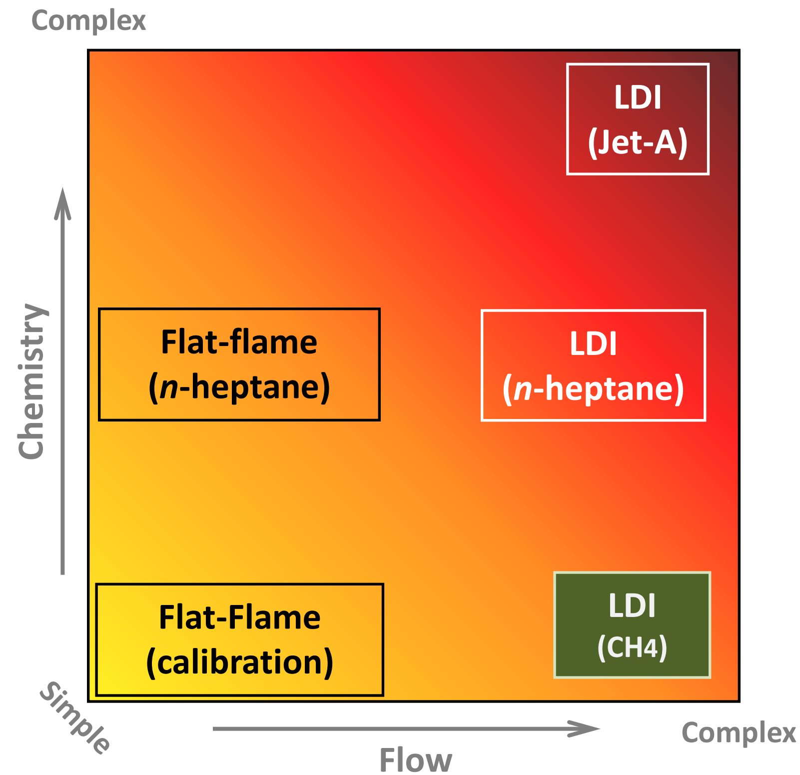
# Approach

**GOAL**

Provide accurate quantitative scalar data for “benchmark tests” for CFD combustor code.

**STRATEGY**

- Advance a point-wise single-shot laser Raman diagnostics
- A series of experiments:
    1. Calibration on reference burners;
    2. Testing on realistic burner;
    3. Increase chemical complexity.



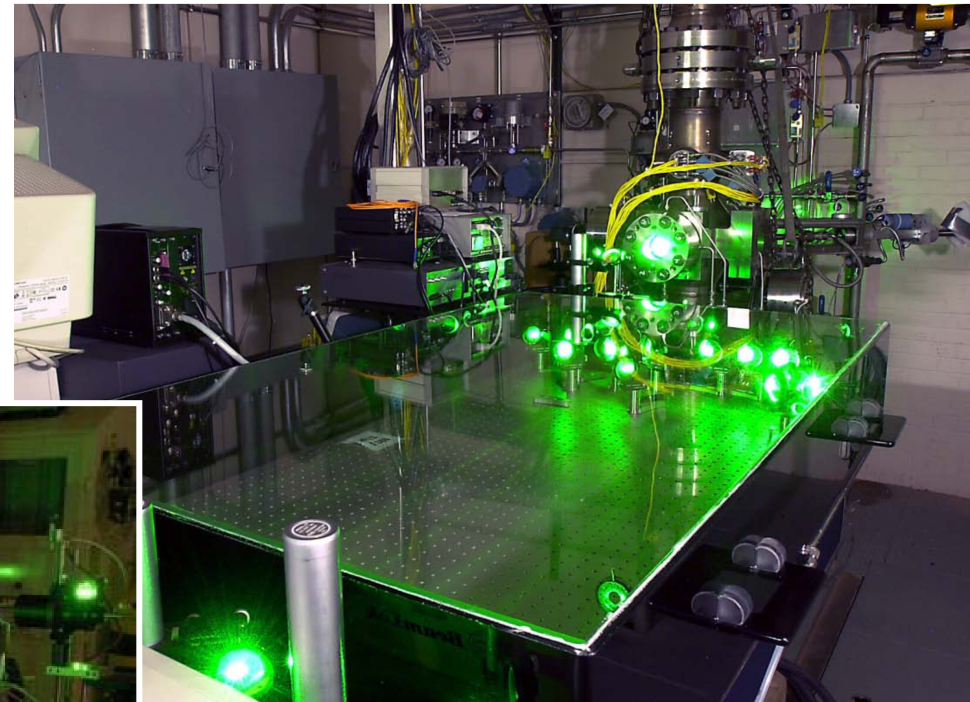

**TECHNICAL CHALLENGE**

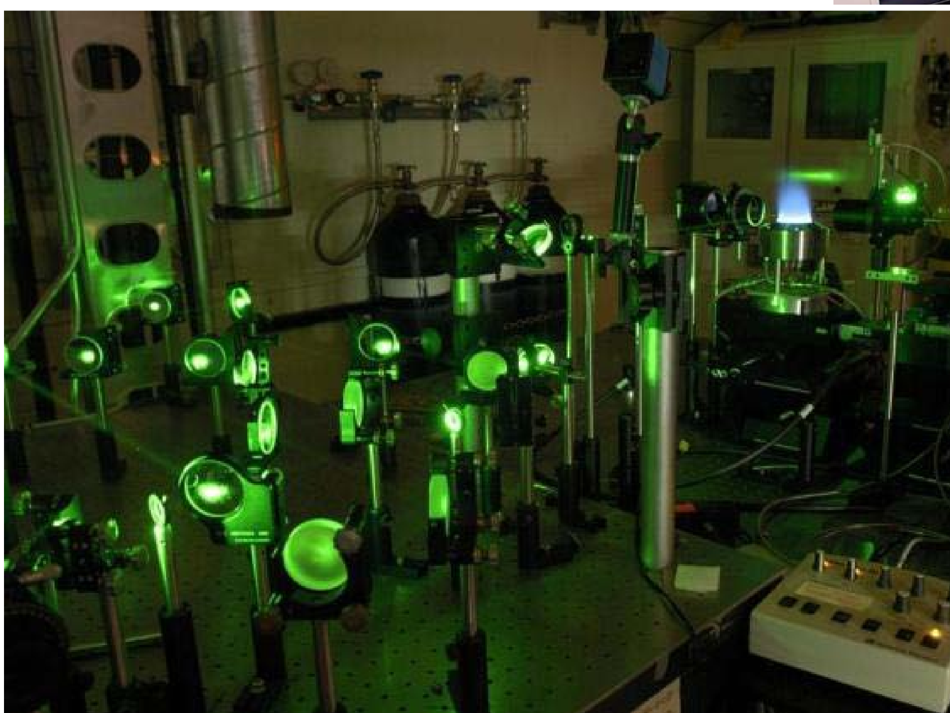
- Simultaneous measurements: temperature, major species, mixture fraction.
- Accuracy: uncertainty <5%.
- Optically-harsh environment: high pressure, geometric limitation, optical interference; two-phase flows.

# Facility

**SE-5** High-Pressure Turbulent Combustion Facility

- Pressure up to 30 atm
- Gaseous and liquid fueled combustion
- Advanced laser diagnostics
- Air can be preheated to 1000F

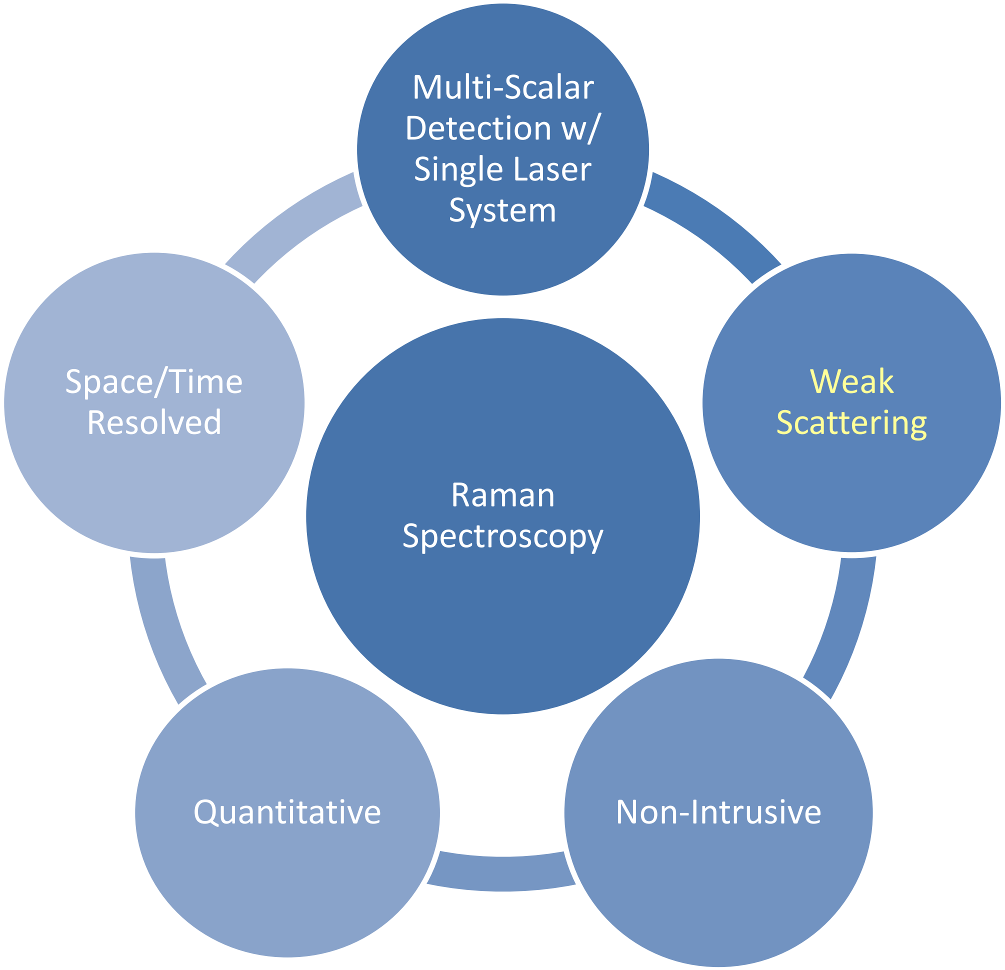




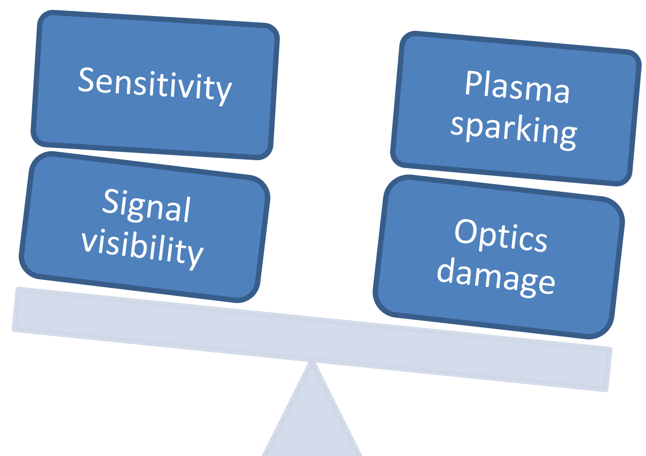
**APCD** Combustion Diagnostics Facility

- Diagnostic development & calibration

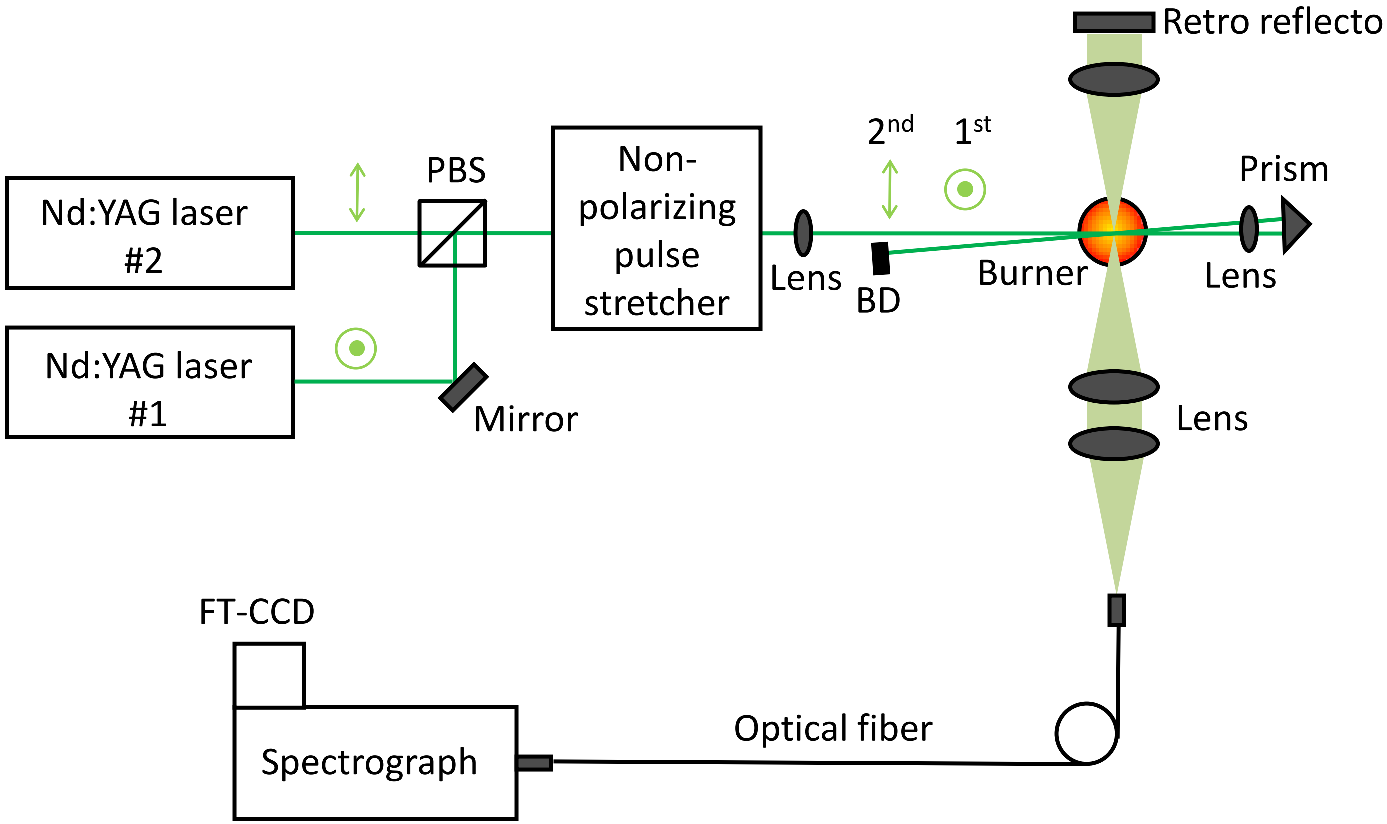
# Linear Raman Diagnostics




*HIGH-POWER PULSED LASER*

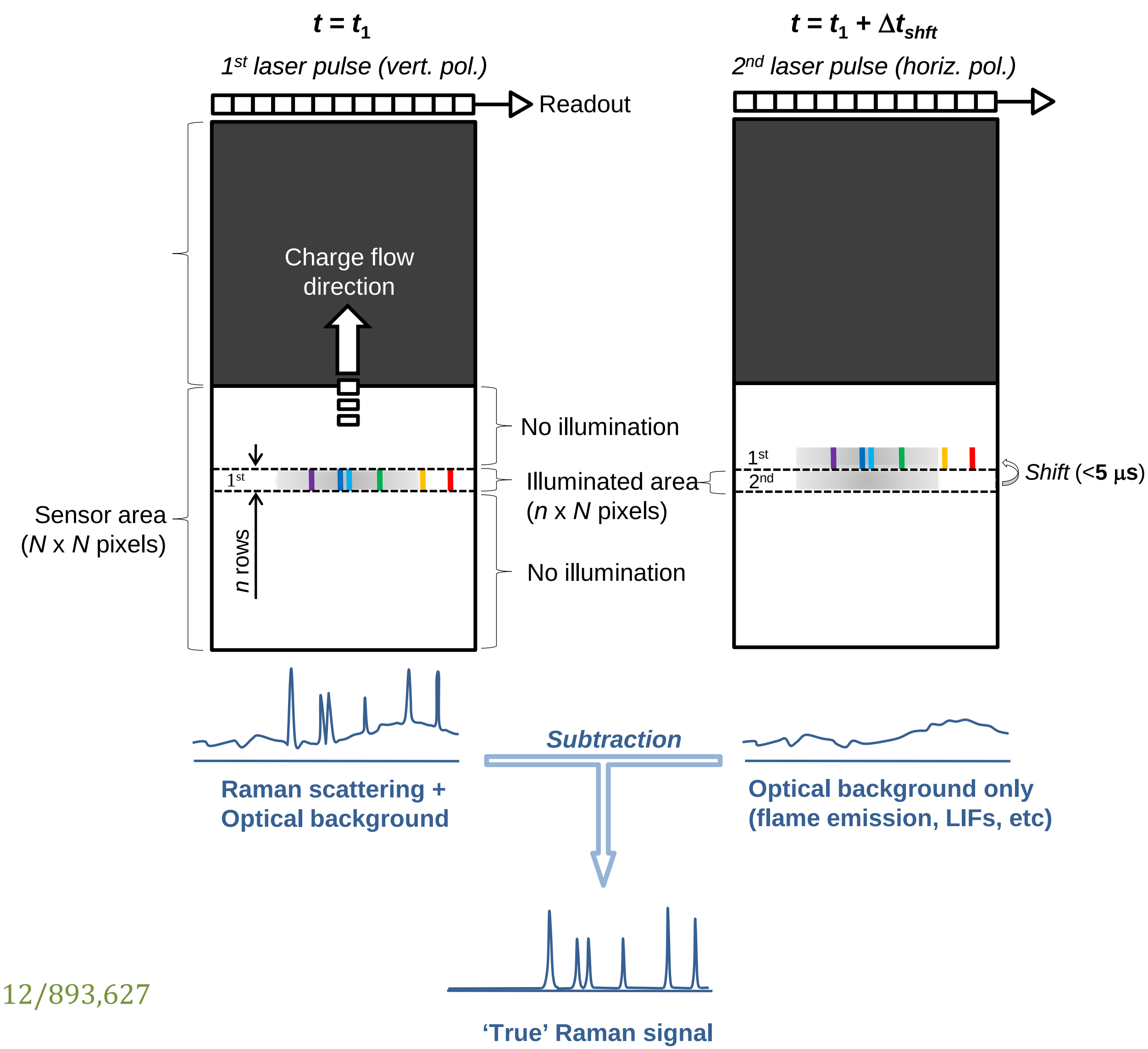


# Interference-free Raman spectroscopy



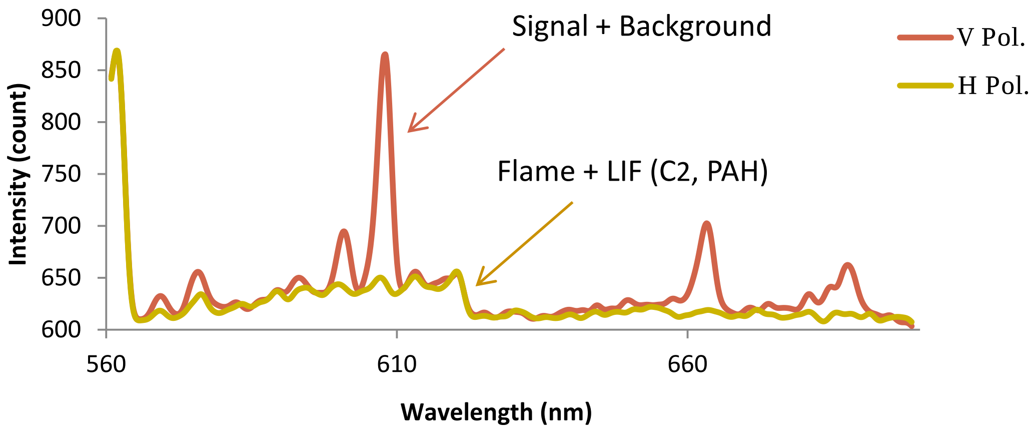

- Developed a patent-pending optical gating scheme: *Subframe Burst Gating (**SBG**).*
- First-ever single-shot polarization-resolved Raman spectroscopy in liquid-fueled combustion, that enabled *interference (noise)-free* scalar measurements.
- Significantly improved signal visibility (5 times) in combustion while eliminating a need of a conventional mechanical shutter for gating.

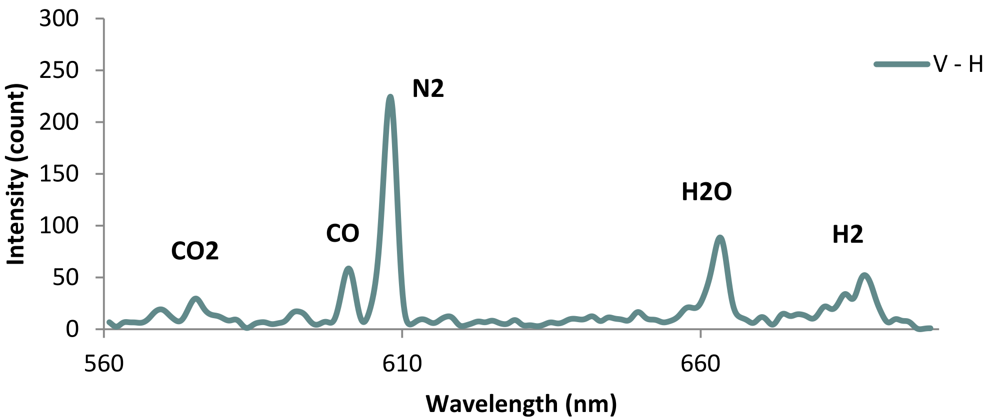
# On-Chip Subframe Burst Gating*




*Patent Application #12/893,627
(filed on 09-29-10)

# Single-shot background-free measurement



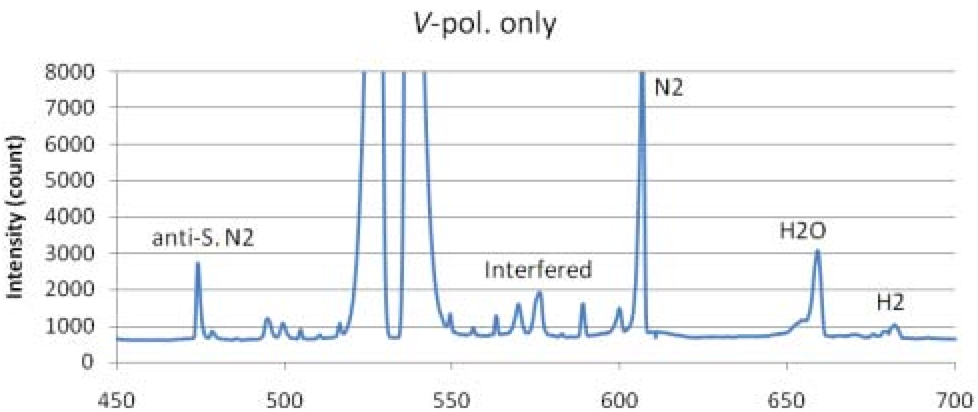



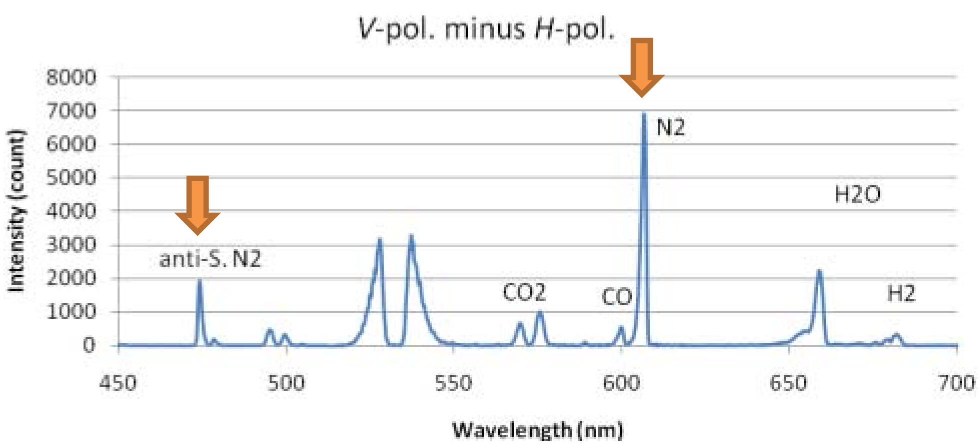

- A fuel-rich n-heptane flame
- A pair of orthogonally-polarized Nd:YAG 532-nm pulsed lasers (650 mJ/pulse)

# Calibration Experiment (I)

## Raman Spectra

$CH_4$/air flames, fuel-rich, Hencken burner,
500-shot averaged




## Species:

*Super-pixel Integration*

| Species | Integration limits (nm) | Integration Width (nm) | Integration Width (pixels) |
|---|---|---|---|
| $CO_2$ ($v_1$,$2v_2$) | 565.5, 578.0 | 12.5 | 48 |
| $O_2$ | 578.0, 581.7 | 3.7 | 14 |
| CO | 596.7, 601.7 | 5.0 | 19 |
| $N_2$ | 601.8, 608.4 | 5.4 | 24 |
| $CH_4$ ($v_1$) | 625.4, 631.9 | 6.5 | 25 |
| $H_2O$ | 644.9, 662.1 | 17.2 | 66 |
| $H_2$ | 662.2., 685.1 | 22.9 | 84 |

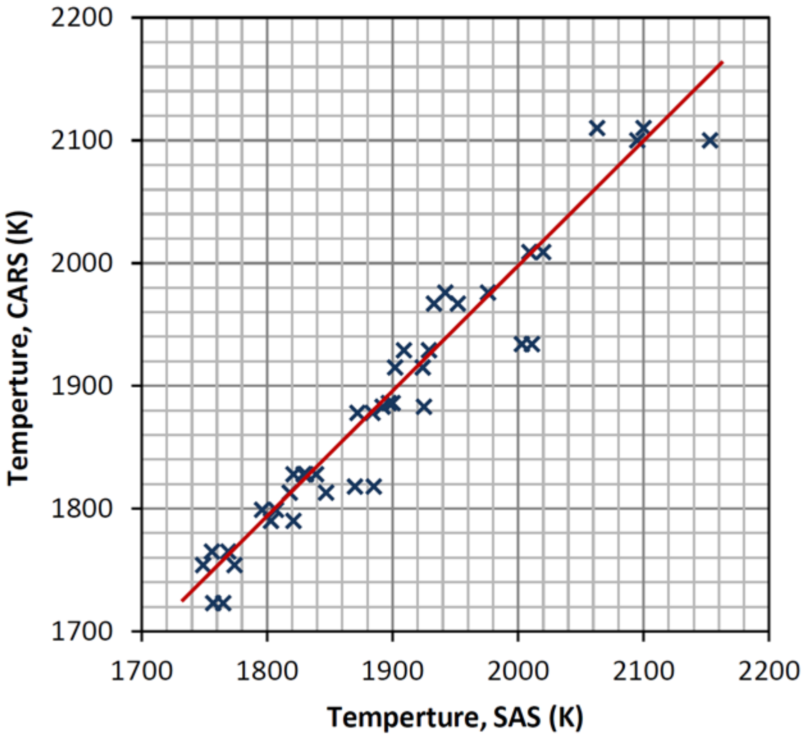
## Temperature:

*Stokes/anti-Stokes ratio of $N_2$*

$$R_{SAS} = \left(\frac{\nu_0 + \nu_s}{\nu_0 - \nu_s}\right) \cdot \exp\left(-\frac{h \cdot c \cdot \nu_s}{\kappa \cdot T}\right)$$

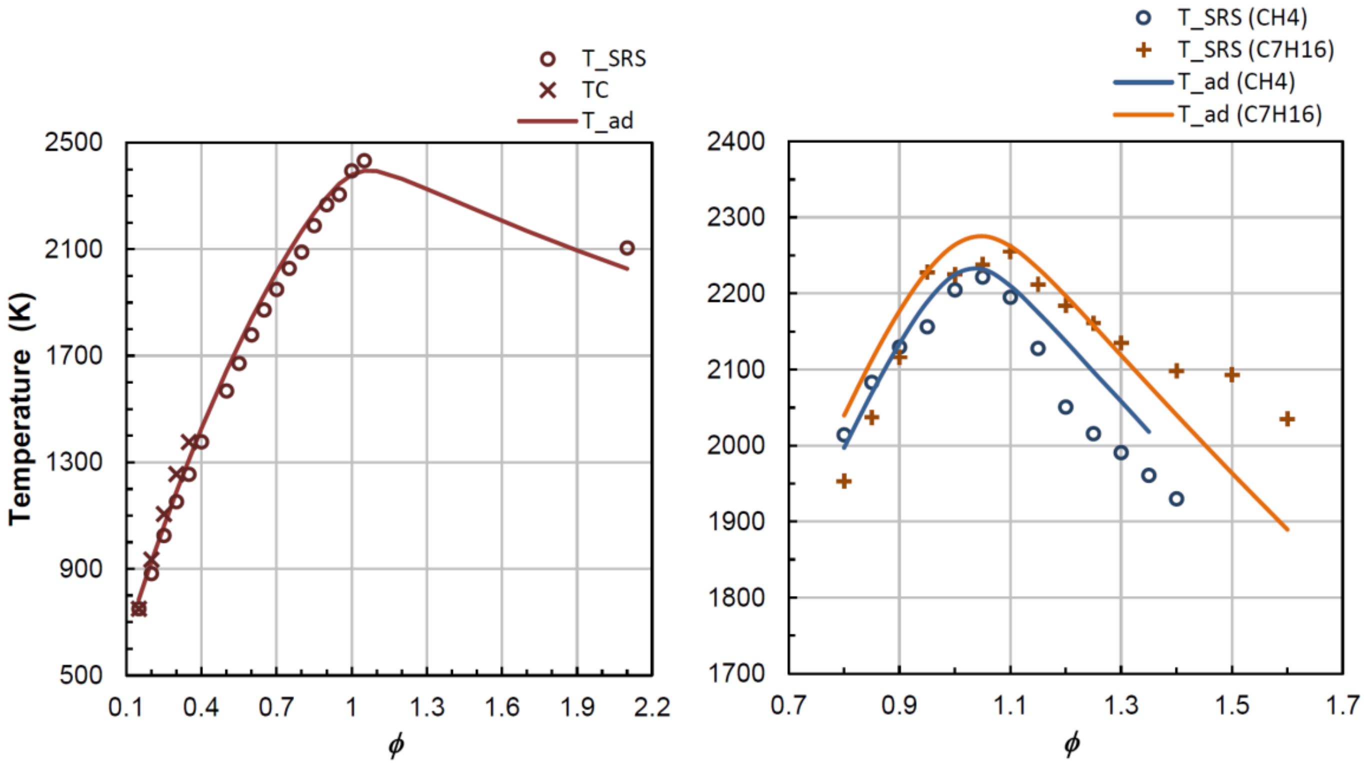
$n_0$: Excitation frequency ($cm^{-1}$); $n_s$: Raman shift ($cm^{-1}$);
$h$: Planck's constant (J/s); $c$: Speed of light (cm/s);
$k$: Boltzmann constant (J/K); $T$: Temperature (K)

# Calibration Experiment (II)



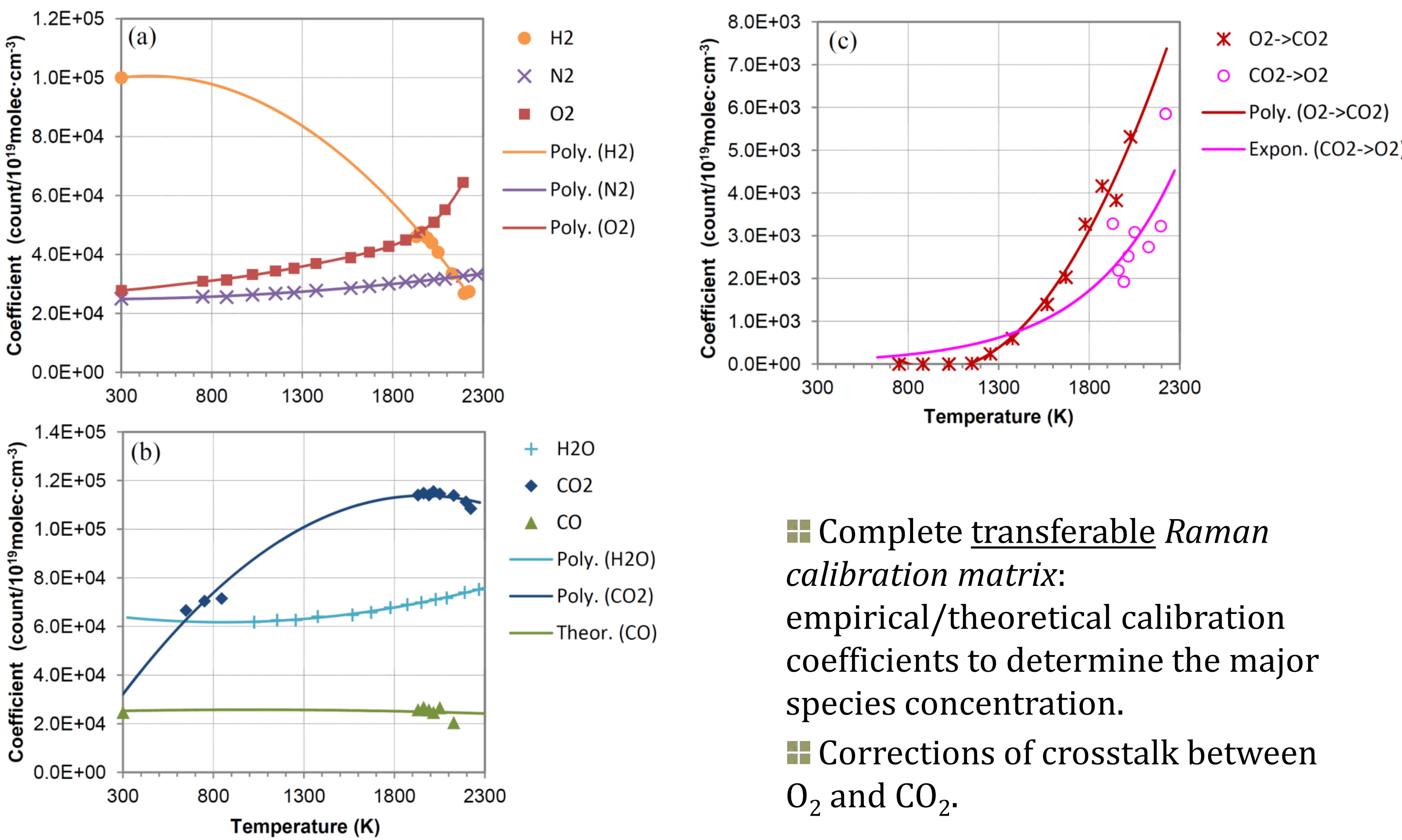

- Diagnostic thermometry cross-check (premixed $CH_4$/air flat-flame)
- Stokes/anti-Stokes (SAS) ratio of $N_2$ vibrational Q-branch band vs. CARS (Meier, DLR)

# Calibration Experiment (III)




- Temperature profiles of the reference standard (calibration) gaseous flames: $H_2$/air flat-flame; $CH_4$/air flat-flame; $C_7H_{16}$/air flat-flame.

# Calibration Experiment (IV)




- Complete <u>transferable</u> *Raman calibration matrix*: empirical/theoretical calibration coefficients to determine the major species concentration.
- Corrections of crosstalk between $O_2$ and $CO_2$.

# Calibration Experiment (V):
## calibration matrix

$$S_i = \Lambda E_L\, k_{i,j}(T)\, N_i$$

$$\boldsymbol{k}_{i,j} = \begin{pmatrix} f(T)_{O2} & 0 & f(T)_{H2\rightarrow O2} & 0 & f(T)_{CO2\rightarrow O2} & 0 \\ 0 & f(T)_{N2} & f(T)_{H2\rightarrow N2} & 0 & 0 & 0 \\ 0 & 0 & f(T)_{H2} & 0 & 0 & 0 \\ 0 & f(T)_{N2\rightarrow CO} & f(T)_{H2\rightarrow CO} & f(T)_{CO} & 0 & 0 \\ f(T)_{O2\rightarrow CO2} & 0 & f(T)_{H2\rightarrow CO2} & 0 & f(T)_{CO2} & 0 \\ 0 & 0 & f(T)_{H2\rightarrow H2O} & 0 & 0 & f(T)_{H2O} \end{pmatrix}$$

$$f(T)_i = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + \cdots + a_n T^n, \text{ or}$$

$$f(T)_i = b_0 \exp(b_1 T)$$

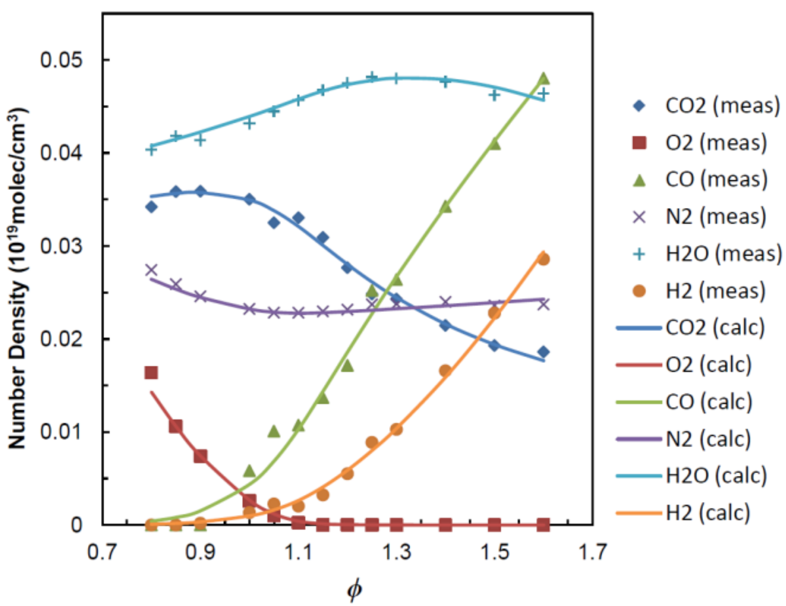
$N_i$: Number density, species $i$
$\Lambda$: Optical throughput/efficiency
$E_L$: Excitation laser energy
$k_{i,j}$: Raman calibration matrix element
$S_i$: Raman scattering signal (super-pixel count)

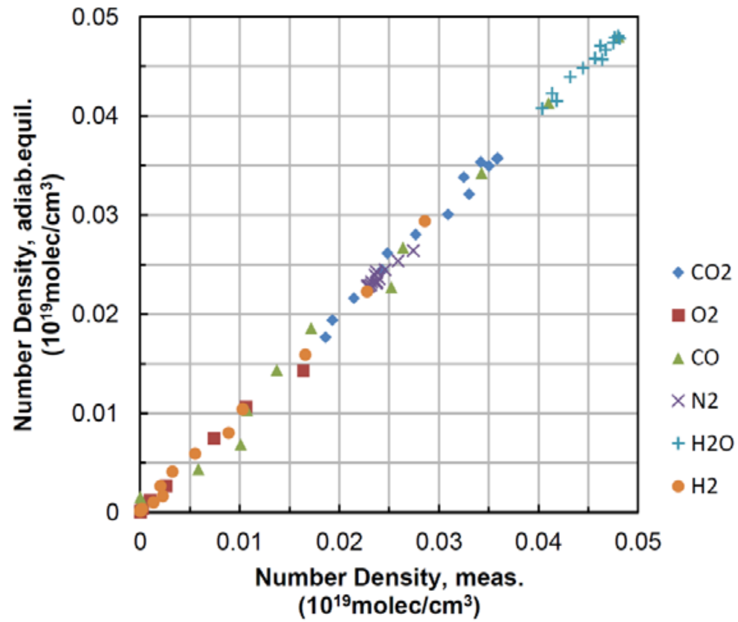
| $k_{ij}$ | $a_0$ | $a_1$ | $a_2$ | $a_3$ | $a_4$ | $a_5$ or $b_0$ | $a_6$ or $b_1$ | Cal. flame |
|---|---|---|---|---|---|---|---|---|
| $CO_2$ | -9.6516E1 | 1.1611E2 | -2.9599E-2 | - | - | - | - | $CH_4$(rich) |
| $O_2$ | 3.0887E4 | -3.4452E1 | 1.2742E-1 | -1.9918E-4 | 1.6531E-7 | -6.8439E-11 | 1.1196E-14 | $H_2$(lean) |
| CO | 2.5515E4 | -1.3450E-1 | 7.0400E-4 | -3.9523E-7 | - | - | - | $CH_4$(rich) |
| $N_2$ | 2.4826E4 | -3.8542E-1 | 1.8054E-3 | - | - | - | - | $H_2$ |
| $CH_4$ | 2.224E5 | - | - | - | - | - | - | cold gas |
| $H_2O$ | 6.6698E4 | -1.1590E1 | 6.7770E-3 | - | - | - | - | $H_2$ |
| $H_2$ | 1.0072E5 | 2.0440 | -1.5094E-2 | - | - | - | - | $H_2$(rich) |
| CO2►O2 | - | - | - | - | - | 4.2732E1 | 2.0524E-3 | $CH_4$(rich) |
| O2►CO2 | -2.0669E3 | 1.1764E1 | -1.9805E-2 | 1.2227E-5 | -2.1984E-9 | - | - | $H_2$(lean) |

# Calibration Experiment (V)

$$N_i = (1/\Lambda E_L)\, k_{i,j}^{-1}(T)\, S_i$$

➢ Inverse matrix formula for N.D. determination

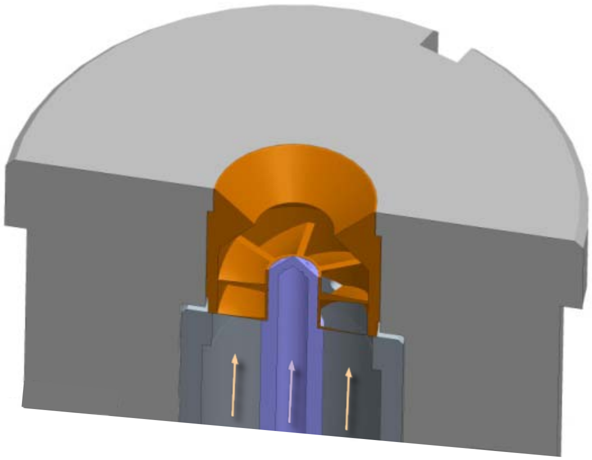


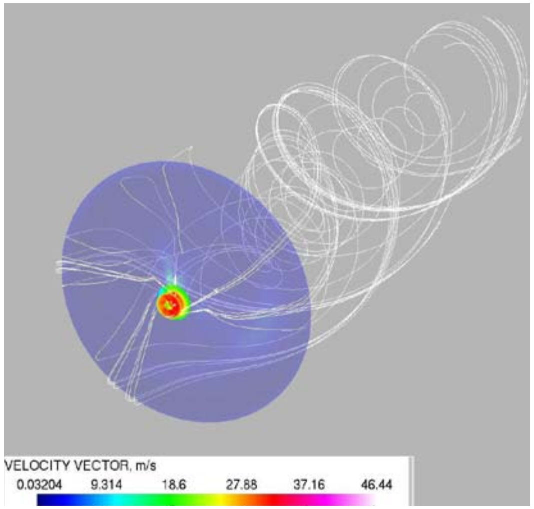




- True scalar value (compared w/ adiabatic chemical equilibrium): $C_7H_{16}$ flat-flame test.
- Measurement accuracy:

| Species | $CO_2$ | $O_2$ | N2 | CO | H2O | H2 |
|---|---|---|---|---|---|---|
| Uncertainty | 2.1% | 6.9% | 1.4% | 8.5% | 1.0% | 5.6% |

# Single-Cup LDI Burner for Validation

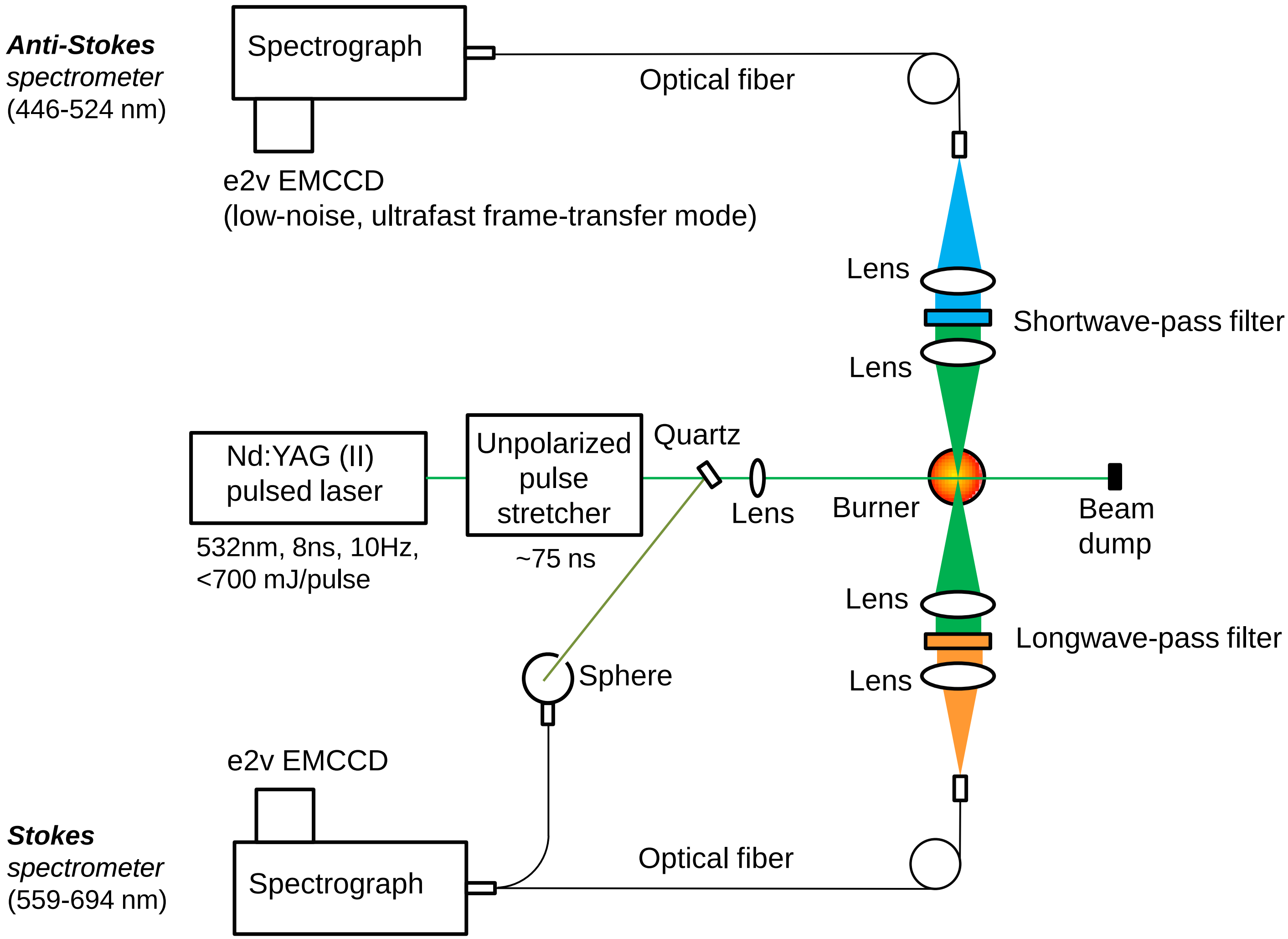




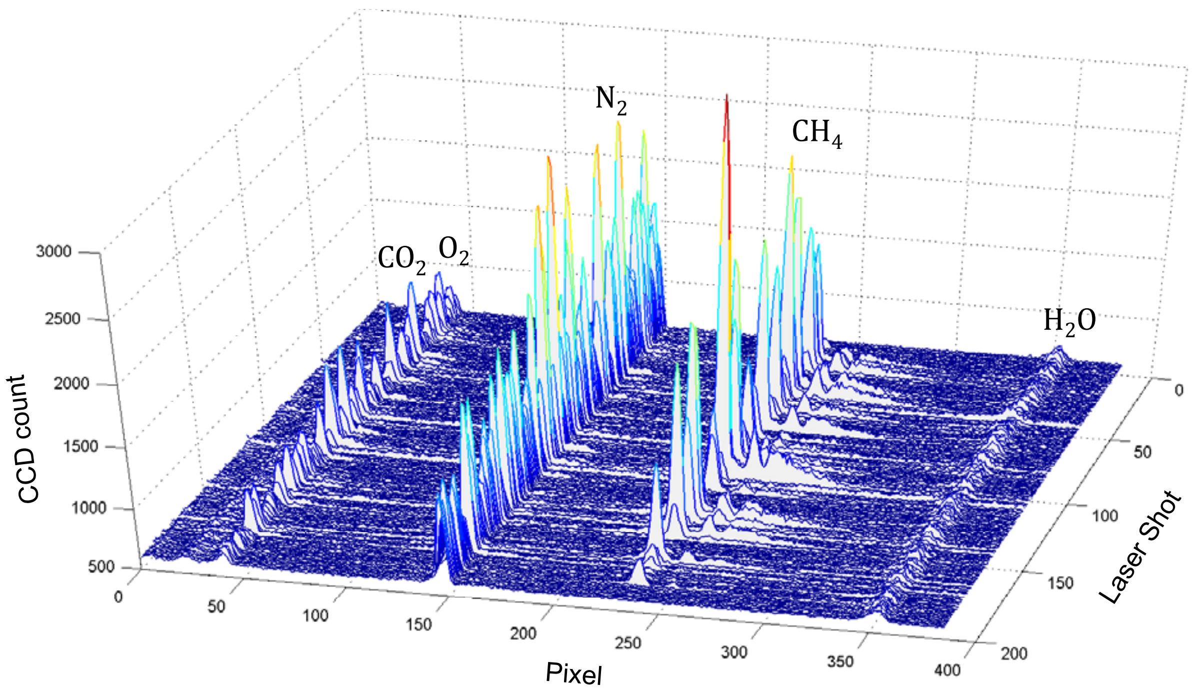

Simulation Credit: C. Wey (RTB)

- Modified angled 6-jet (1 mm dia. each) gaseous fuel Lean-Direct Injection
- CFD friendly design
- Interchangeable between gaseous and liquid fuel injectors
- Swirler (1” cup): 60-deg and 45-deg.
- Latest run: $\Phi$ = 0.74, $P$ = 250 psia, 940 slm air.

# Raman Diagnostics Setup (point-wise):
## New Dual-SBG Detection

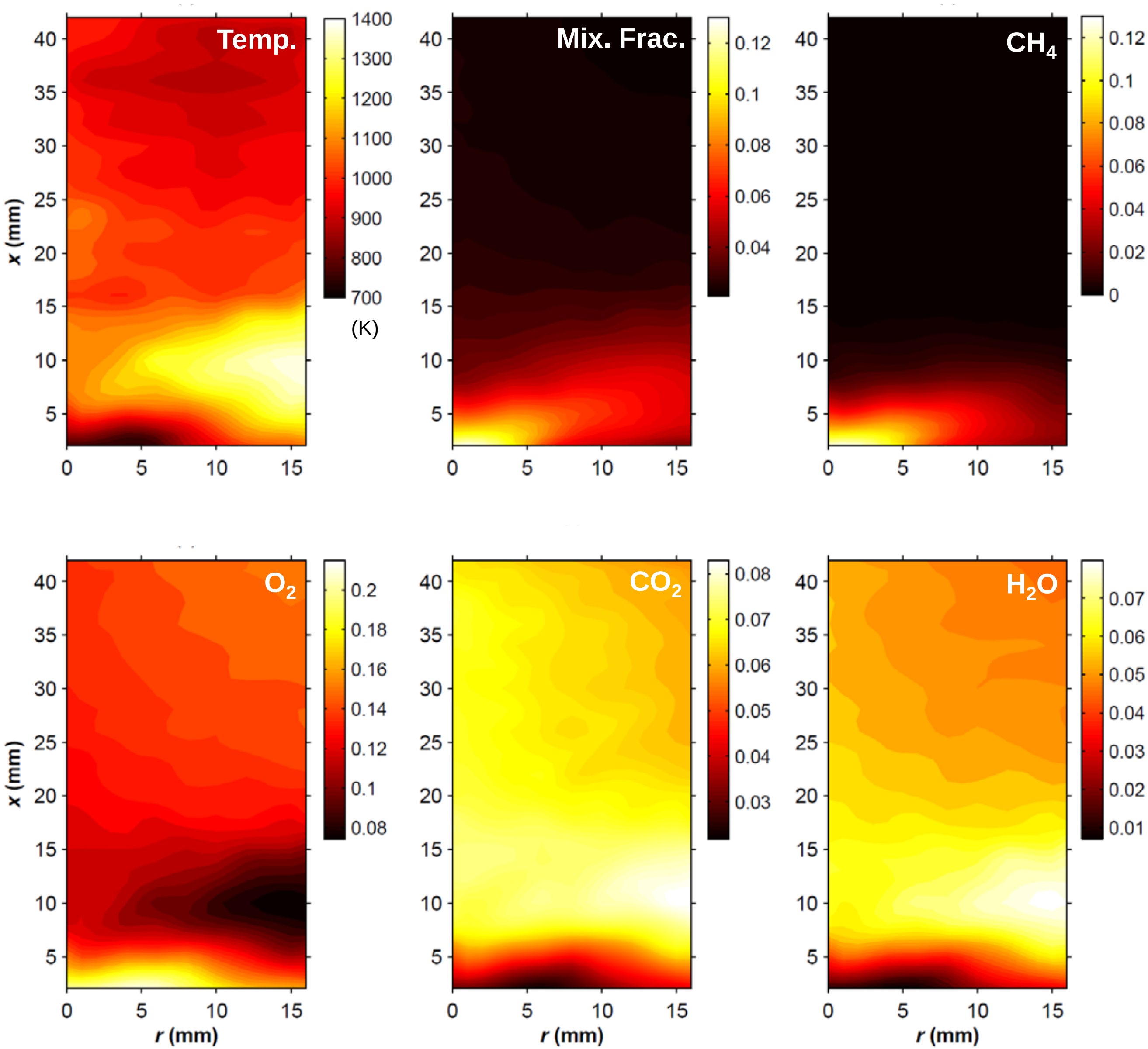


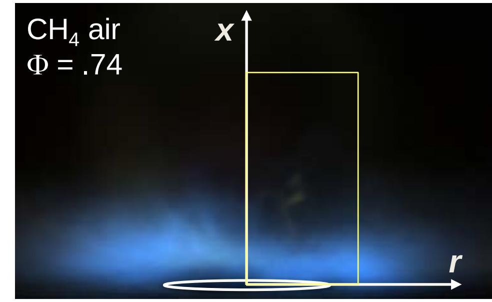
# Single-Shot Raman Spectra




- Raw spectral data (10-Hz repetition rate).
- Raman frequency signature $\rightarrow$ Chemical composition
- Random changes in intensity $\rightarrow$ Turbulent mixing
- Simultaneous measurements of multiple variables $\rightarrow$ Combustor code validation

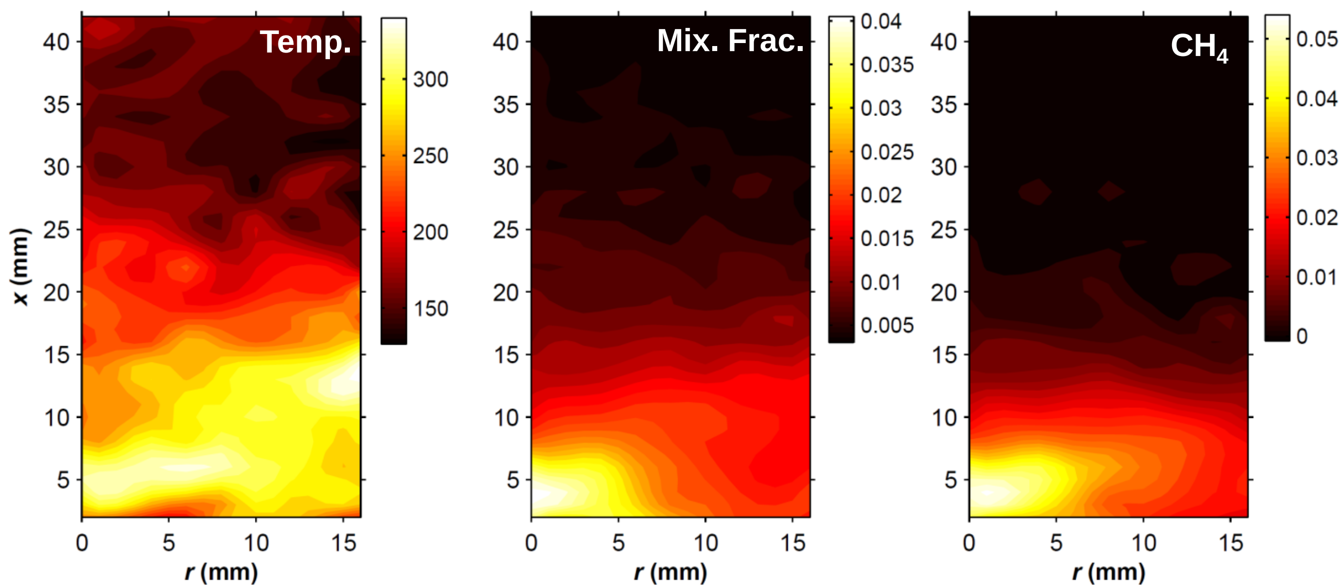
# Scalar Contour (averaged)



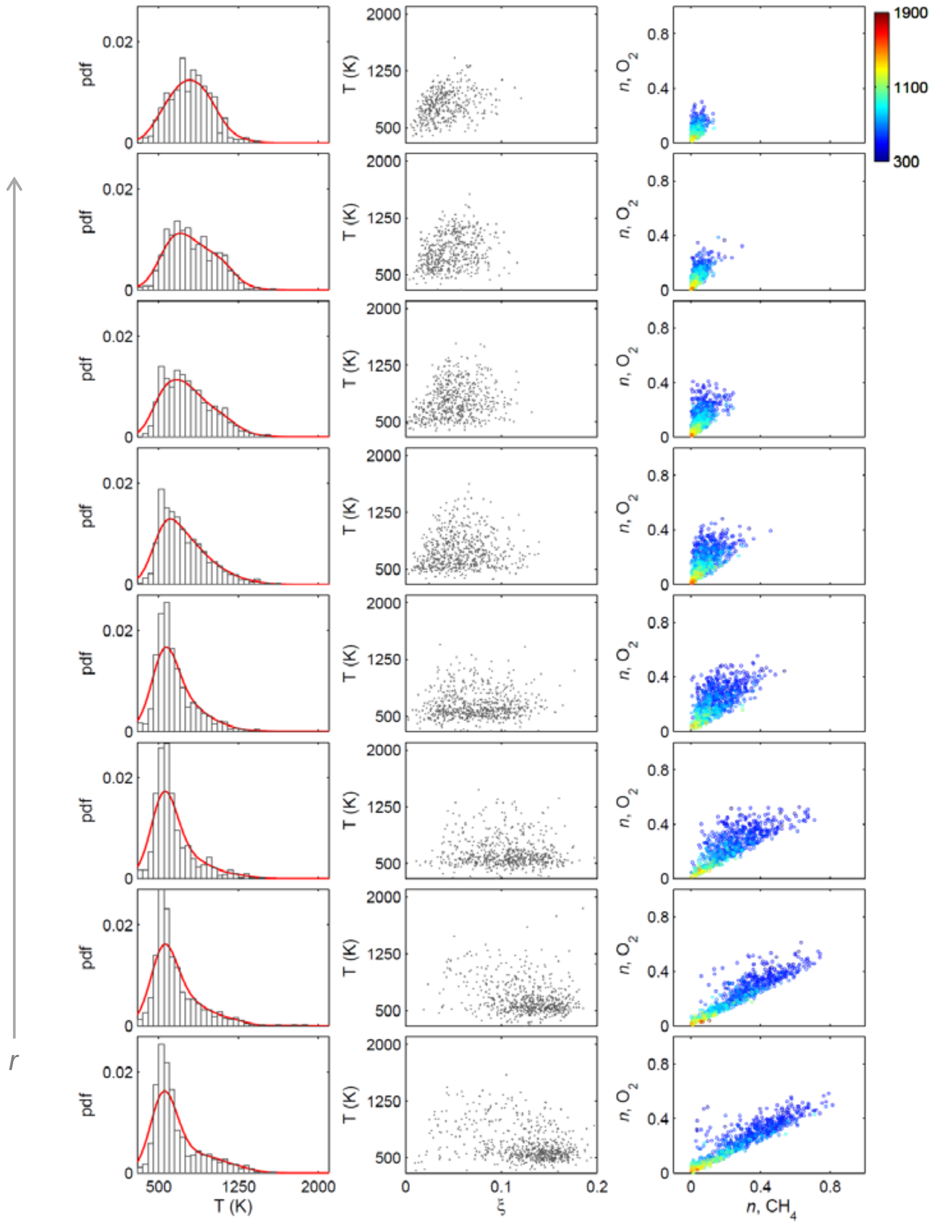

- Temp: ave. low 700 K; ave. high 1400 K.
- Side-spreading, low-profile flame (indicated by the temp).
- Majority of mixing within 8 mm height.
- Almost no residual fuel above 15 mm height.
- Predictable $CO_2$, $H_2O$ (combustion product) profiles in post-flame zone.

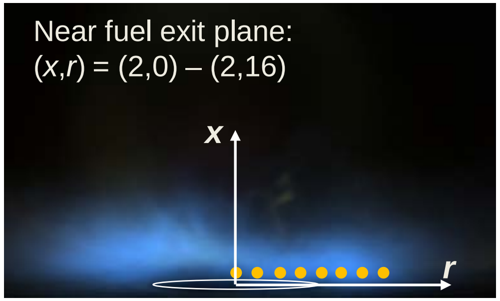
# Scalar Contour (standard deviation)




- Temp RMS shows the region with swirl-induced turbulent-chemistry interaction.
- Mixture fraction and fuel RMS support the idea.

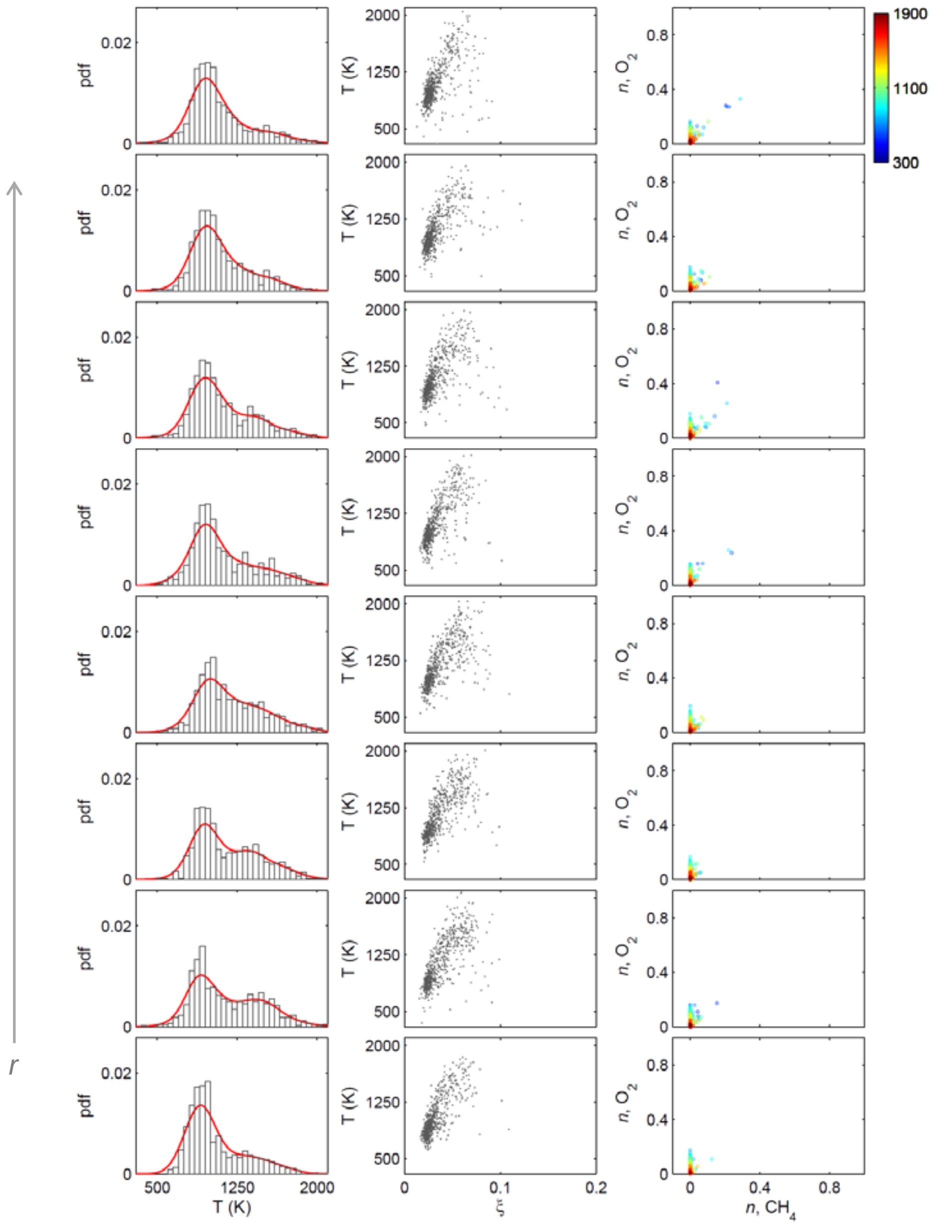
# Thermochemical Analysis (I)

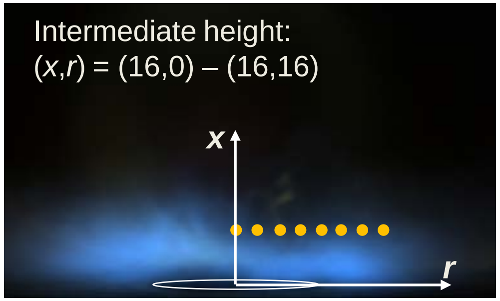



- Highly turbulent (mixing) region indicated by the largest scatter in mixture fraction (scatter plots).
- Reaction incomplete (3-scalar correlation).
- Co-existence of *cold* fuel and oxidizer – unburnt pockets.

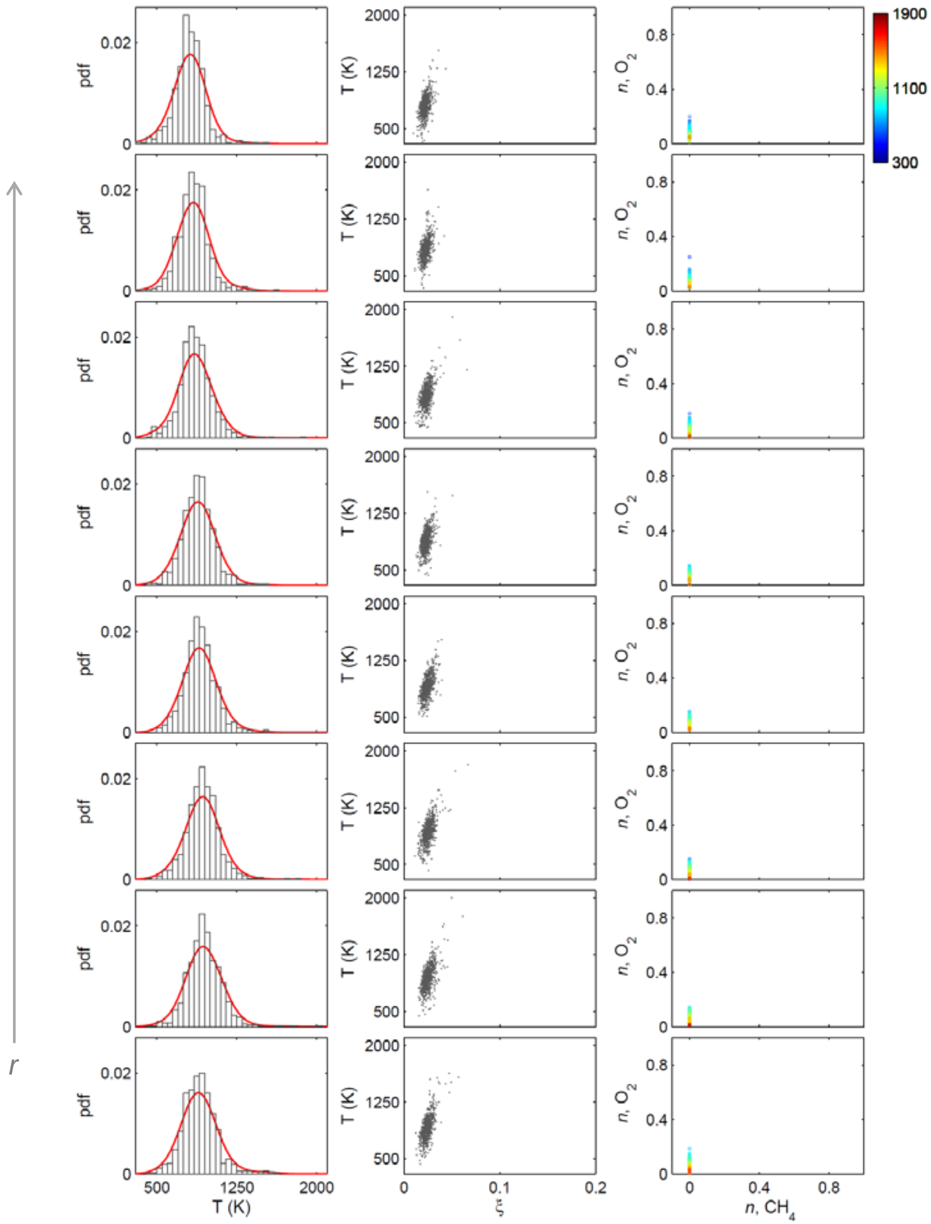
# Thermochemical Analysis (II)

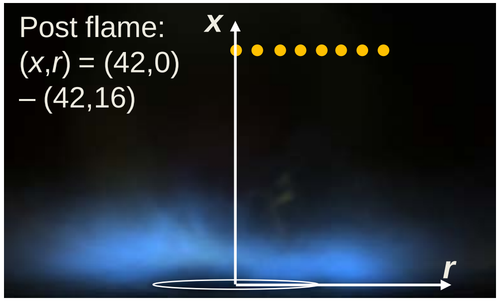



- Reaction zone: reached at the highest temp (approx. 2000K with the widest temp distribution (PDF/scatter plot).
- Unique bimodal distribution (PDF) – recirculation zone.
- Little fuel residual (3 scalar correlation).

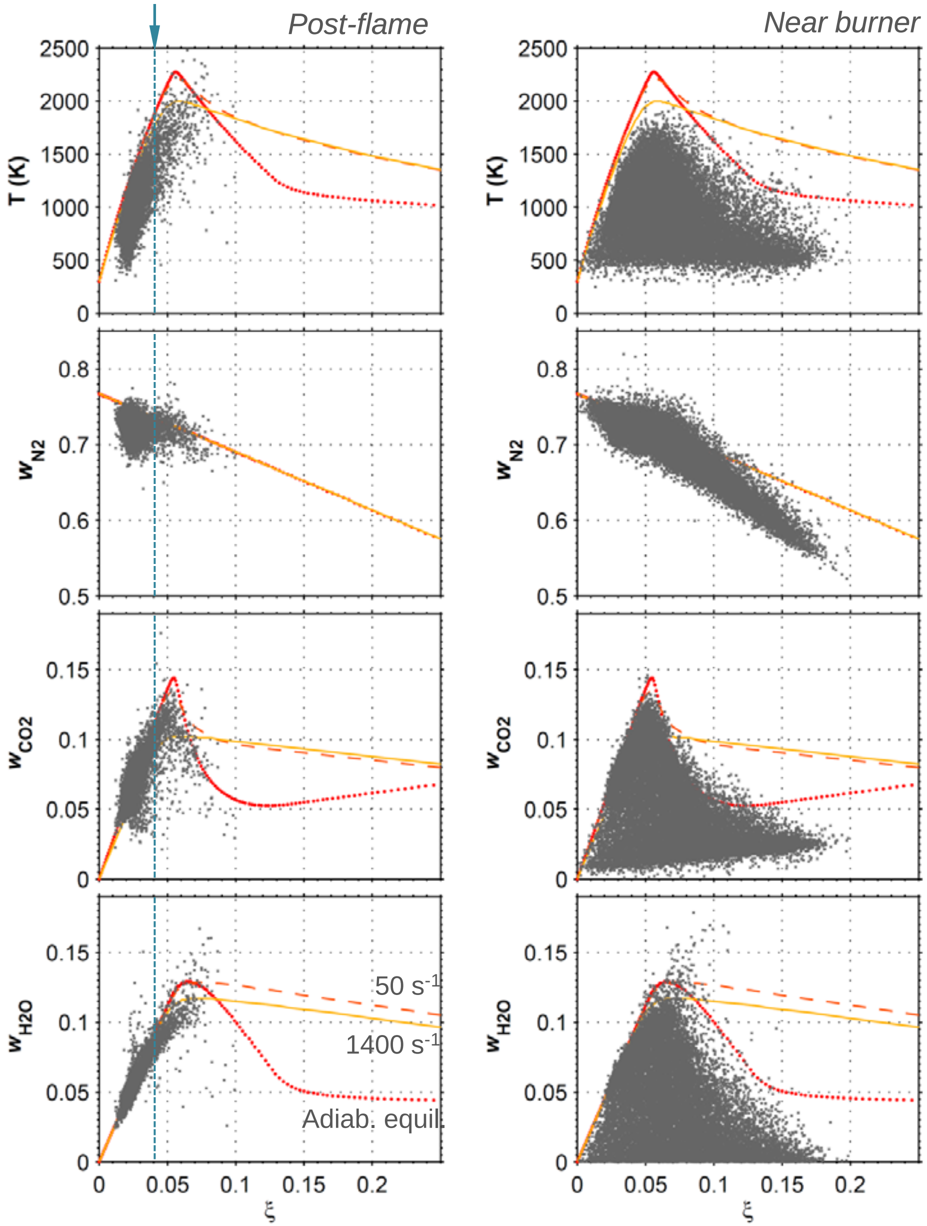
# Thermochemical Analysis (III)



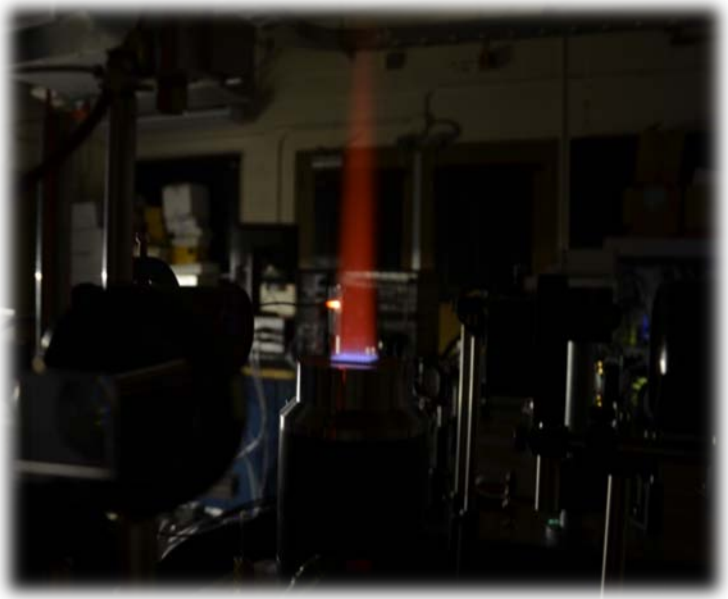

- Post-flame zone: homogeneous, well-reacted region indicated by normal (narrower) distribution.
- No residual fuel.
- Very little scatter in mixture fraction (end of fuel-air mixing)

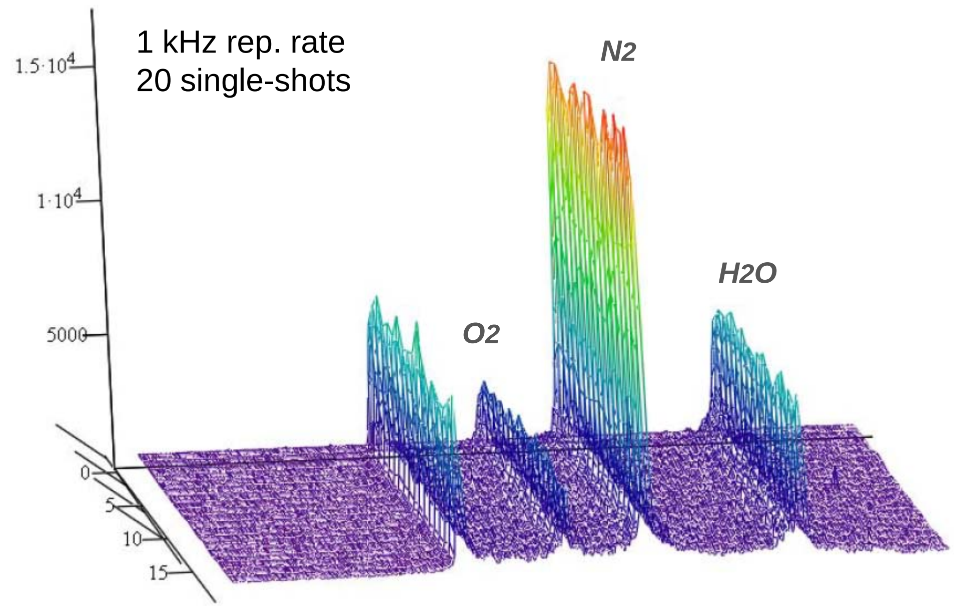
# Thermochemical Analysis (IV)




- Overall profile agreement with laminar flame calculation (UC Berkely) – precision of the measurement.
- Large number of samples (mixing and reaction zone) out of adiabatic equilibrium condition – nature of non-premixed turbulent flames.
- Dominant partially premixed combustion regime.
- A majority of the measured samples (at the post flame zone) indicated complete or near-complete reaction.
- Mixing-only conditions (i.e., preheated to below-ignition-point temperature) following the global equivalence ratio of the flame: Evidence of fast premixing.

# High-Speed Raman Scattering Measurements






- Diagnostics for combustion dynamics and instability.
- Demonstration in a fuel-lean $H_2$-air flat-flame.
- Single-shot Raman spectra at 1 kHz data rate with a 527-nm DPSS Nd:YLF laser (30 mJ/pulse, 30W) and a high-speed image-intensified CCD camera.
- Trade-off: data rate vs. accuracy
- 10-kHz system under development.

# Summary

✓ Significant upgrade to SE5 high-pressure turbulent combustion validation facility (nasa grc): available for code-validation experiments.

✓ Unconventional laser Raman diagnostics (double-SBG) is invented for routine operations.

✓ Generated one-of-the-kind quantitative multi-scalar data for swirl-stabilized combustion at 250 psia (17 atm).

✓ Our thermochemical analysis explored nature of the turbulent flame structure.