ABSTRACT
In support of NASA ARMD's code validation project, we have made significant progress by providing the first quantitative single-shot multi-scalar data from a turbulent elevated-pressure (5 atm), swirl-stabilized, lean direct injection (LDI) type research burner operating on CH4-air using a spatially-resolved pulsed-laser spontaneous Raman diagnostic technique. The Raman diagnostics apparatus and data analysis that we present here were developed over the past 6 years at Glenn Research Center. From the Raman scattering data, we produce spatially-mapped probability density functions (PDF’s) of the instantaneous temperature, determined using a newly developed low-resolution effective rotational bandwidth (ERB) technique. The measured 3-scalar (triplet) correlations, between temperature, CH4, and O2 concentrations, as well as their PDF’s, also provide a high-level of detail into the nature and extent of the turbulent mixing process and its impact on chemical reactions in a realistic gas turbine injector flame at elevated pressures. The multi-scalar triplet data set presented here provides a good validation case for CFD combustion codes to simulate by providing both average and statistical values for the 3 measured scalars.
Single-Shot Scalar-Triplet Measurements in High-Pressure Swirl-Stabilized Flames for Combustion Code Validation

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H2-Air Flame at 20 atm

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Overview

**Goal:** Provide critical chemical and physical data in turbulent combustion at realistic subsonic/supersonic cruise condition for **validating predictive low-emissions combustor codes**

**Challenges:** Successful accurate multiscalar measurements (temperature, major species mole fractions, mixture fraction, velocity) in optically-harsh droplet-laden flows at **high pressures**.

**Strategy (tasks):**

- Develop a quantitative time-resolved **laser Raman diagnostics**
- A series of experiments of increasing flow complexity: (i) Calibration burner (e.g., flat-flame burner), (ii) Realistic concept burners (swirl-stabilized burner) at **elevated pressures** up to 10~30 atm
- Address the effects of chemical complexity: $\text{H}_2$, $\text{CH}_4$, single-component liquid (e.g., hexane, iso-octane, n-heptane), jet-A fuel
Atmospheric Pressure Combustion Diagnostics Facility

- Temperature and species reference
- Diagnostics calibration
- Gaseous fuels
- Pre-vaporized single-component liquid fuel (electronically controlled fuel vaporizer and heating system)
- Support visible and UV laser Raman systems
- Study on optical characteristics of sooting flames and liquid fuel combustion chemistry
- Support the Aeronautics milestones to mitigate risks due to PSO holding up high-pressure experiments
High Pressure Burner Facility (SE-5)

- Remotely controlled with auto process controller
- Pressure up to 30 atm (currently 10 atm requested for safety permit)
- Versatile for burner platform (calibration burner, turbulent jet, LDI)
- Optical access (4 ports)
- Gaseous and liquid fuel capacity
- Air pre-heater installed (up to 1200F)
Raman Scattering Diagnostic System

- Nd:YAG Laser (800 mJ/pulse)
- Laser Pulse-Stretcher (passive multiple ring-cavity) *Patent pending
- Beamsplitters
- Mirrors
- High-Pressure Rig
- Burner
- Folding Prism
- Optical Fibers
- Electro-mechanical high-speed shutter *2007 R&D 100 Award
  - 10’s μs gate width
- Laser line filter
- CCD
  - 1340 x 100 pixels
  - 90% Q.E.
  - 16 bit A/D
- Holographic spectrograph (f/1.8)

Graph showing intensity vs. time for original and stretched pulses.
Raman Spectra Observed in Combustion

**Advantage**
- Raman scattering – simultaneous multiple species concentration and temperature
- Time-average (mean) or Single-shot (instantaneous; rms)
- Quantitative

**Challenge**
- Spectral interference (‘Cross-talk’)

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**Excitation**

- H₂-air flame (10 atm, fuel-rich)
- Rotational N₂/O₂
- (CO)
- CH₄
- H₂O

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**Wavelength (nm)**

- 450
- 500
- 550
- 600
- 650
- 700

**Intensity (a.u.)**
Raman Calibration Experiments & Simulation

**Platform**
- Static cell
- Calib. burner

**Fuel**
(lean ~ rich)
- H₂
- H₂-CO
- CH₄
- Single-component liquid (pre-vaporized)
- Single-component liquid
- Multi-component liquid (jet-A)
- Air

**Raman Instrumentation**
- Pump lasers: 532/355/266 nm
- Thermometry: Vib. / Rot.
- Polarization property

**Matrix elements, \( k_{ij}(T) \)**
(Cross-talks)
- Major species (H₂, O₂, N₂, CO, CO₂, H₂O, HC’s)
  - H₂ → CO
  - H₂ → CO₂
  - H₂ → H₂O
  - N₂ → CO
  - O₂ → CO₂
  - CO₂ → N₂
  - C₂* → N₂, CO, HC’s
  - PAH → Broadband background
Determine the ‘Cross-talk’ Calibration Matrix

**Raman Spectra Library**

- Calibration matrix
  \[
  N_i = \left(\frac{1}{E_{\text{laser}}}\right) k_{ii}(T) S_i
  \]

**Calibrated Results**

- Mole frac.
- Calibration factor \(10^{19} \text{ molecules cm}^{-1} \mu\text{W}^{-1}\text{nm}^{-1}\)
- 10 atm, \(\text{H}_2\)-air flame

**Experiments or Simulations**

- Fuel-Lean
- Fuel-Rich
NASA Lean Direct Injection (LDI) Swirl-Stabilized Research Burner — Preliminary Test —

- Swirl-stabilized direct fuel injection design (gaseous)
- Integrated with existing high-pressure rig
- 6 jets (0.8 mm in dia.) angled at 45 deg to burner axis
- Initial test on H₂ and CH₄ fuels with unheated air at 5 atm
- Collaborating with National Combustor Code (NCC)
Single-Shot (Time-Resolved) Raman Measurements

• One shot = One instance (space-time point)
• Single-shot Raman data shows “random” change due to turbulence
• Direct and simultaneous measurement of fuel/oxidizer concentrations and temperature (with data processing with calibration matrix)
• Developed new thermometry approach (rot. bandwidth) with high SNR

Temperature from the rotational spectra has been measured with accuracy 7%

Data permits statistical PDF’s of temperature and species

Provides a signature for characterizing degree of mixing and reaction
Processing the Single-Shot Data

Number density $[10^{19} \text{ molec/cm}^3]$
Probability Density Functions: PDF’s
(Temperature, CH₄, and O₂)

CH₄-air LDI flame (5 atm, Phi = 0.5)

- Spatially-mapped multi-scalar PDF “library” in given conditions provides excellent validation data for a predictive combustion code.

- Difference between mean and distribution (statistical value)

Averaged value
Multiscalar Analysis in 5-atm CH₄-Air LDI Flame

‘Production-mode’ data
: Direct output from a MATLAB code

1. Temperature PDF’s
2. Temp. vs species correlations
   (red: O₂; blue: CH₄)
3. Triplet correlations (temp-ox-fuel)
   (with a global Phi of 0.5 line)

Data interpretation
✓ Hot spots (high NOx)
✓ Unique bi-modal PDF’s — recirculation zone, or combustion oscillations
✓ Turbulent-chemistry interaction
✓ Fuel-air mixing characteristics
✓ Unburnt pockets
Multiscalar Analysis in 5-atm CH₄-Air LDI Flame

Data interpretation

✓ Gaussian-like narrow Temp. distribution (centered around the adiabatic temp. at Phi of 0.5)
✓ No fuel (CH₄) residual = fully consumed
✓ No hot or cold spots
✓ Homogeneous, well-reacted post-flame zone
Conclusions

• A single-shot (time-resolve) capability of a laser Raman diagnostics has been confirmed.

• Preliminary data of time-resolved multiscalar data in a high-pressure (turbulent) swirl-stabilized flame has been acquired.

• A new single-shot data-processing scheme (computer code) has been developed for ‘production mode’ thermo-chemical analysis.

• Scalar PDF’s and 3D (temp-oxy-fuel) correlations showed promising capability of future use in code validation.

Work-in-progress

• APCD (atmospheric pressure combustion diagnostics) facility is under construction to calibrate and improve the Raman diagnostics applicable to liquid fuels.

• Modified visible and UV Raman diagnostic systems is under development to cope with harsh environments.

• Computer code to simulate Raman spectra of major species including CO₂ and H₂O (except hydrocarbon) is under development to complete the calibration matrix.

• Pressure Safety Office safety permits, variances in process.