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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**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: H₂, CH₄, 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*
- **OAI** (Ohio Aerospace Institute)
- **Image**: Original pulse and stretched pulse graph
- **Graph Details**:
  - Intensity (a.u.)
  - Time (nano seconds)
- **Equipment**:
  - High-Pressure Rig
  - Burner
  - Folding Prism
- **Optical Components**:
  - Beamsplitters
  - Mirrors
  - Electro-mechanical high-speed shutter
    *2007 R&D 100 Award*
    - 10’s μs gate width
  - Optical Fibers
  - Laser line filter
  - Holographic spectrograph (f/1.8)
- **CCD**:
  - 1340 x 100 pixels
  - 90% Q.E.
  - 16 bit A/D
- **PC**
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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**Graph:**
- **Excitation (532 nm)**
- **Wavelength (nm):** 450, 500, 550, 600, 650, 700
- **Intensity (a.u.):**
- **Species:** H\textsubscript{2}-air flame (10 atm, fuel-rich), Rotational N\textsubscript{2}/O\textsubscript{2}, N\textsubscript{2}, CO\textsubscript{2}, O\textsubscript{2}, CH\textsubscript{4}, H\textsubscript{2}O
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 (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 \( \rightarrow \) CO
  - H₂ \( \rightarrow \) CO₂
  - H₂ \( \rightarrow \) H₂O
  - N₂ \( \rightarrow \) CO
  - O₂ \( \rightarrow \) CO₂
  - CO₂ \( \rightarrow \) N₂
  - C₂* \( \rightarrow \) N₂, CO, HC’s
  - PAH \( \rightarrow \) Broadband background

Raman spectrum simulation
Determine the ‘Cross-talk’ Calibration Matrix

Raman Spectra Library

Calibration matrix

Mole frac.

\[ N_i = \left( \frac{1}{E_{\text{laser}}} \right) k_{i,j}(T) S_i \]

Calibrated Results

Experiments or Simulations

- \( N_2 \)
- \( H_2 \)
- \( O_2 \)
- \( CO \)
- \( CO_2 \)
- \( H_2O \)
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

Rotational N2 Raman band

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Normalized intensity (a.u.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T = 500 K</td>
<td>1</td>
</tr>
<tr>
<td>T = 1500 K</td>
<td>0.5</td>
</tr>
<tr>
<td>T = 2500 K</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Raman shift (or wavelength)
Processing the Single-Shot Data

Number density
$[1.019 \text{ molec}/\text{cm}^3]$
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)
Multiscalar Analysis in 5-atm CH\textsubscript{4}-Air LDI Flame

*Production-mode* data

: Direct output from a MATLAB code

1. Temperature PDF’s
2. Temp. vs species correlations (*red*: O\textsubscript{2}; *blue*: CH\textsubscript{4})
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.