

Reaction Zone Detection and Characterization in Partially Premixed Flames

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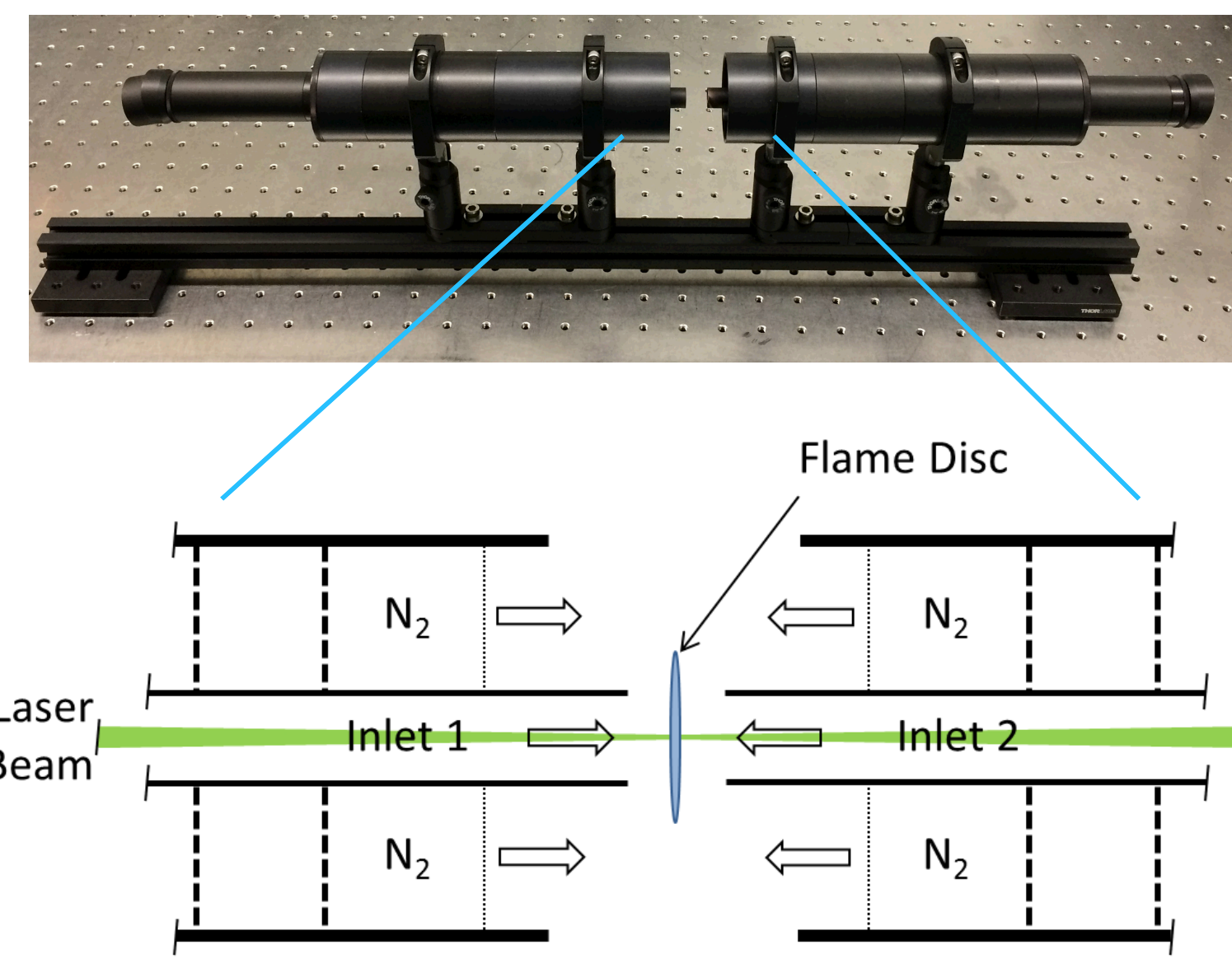
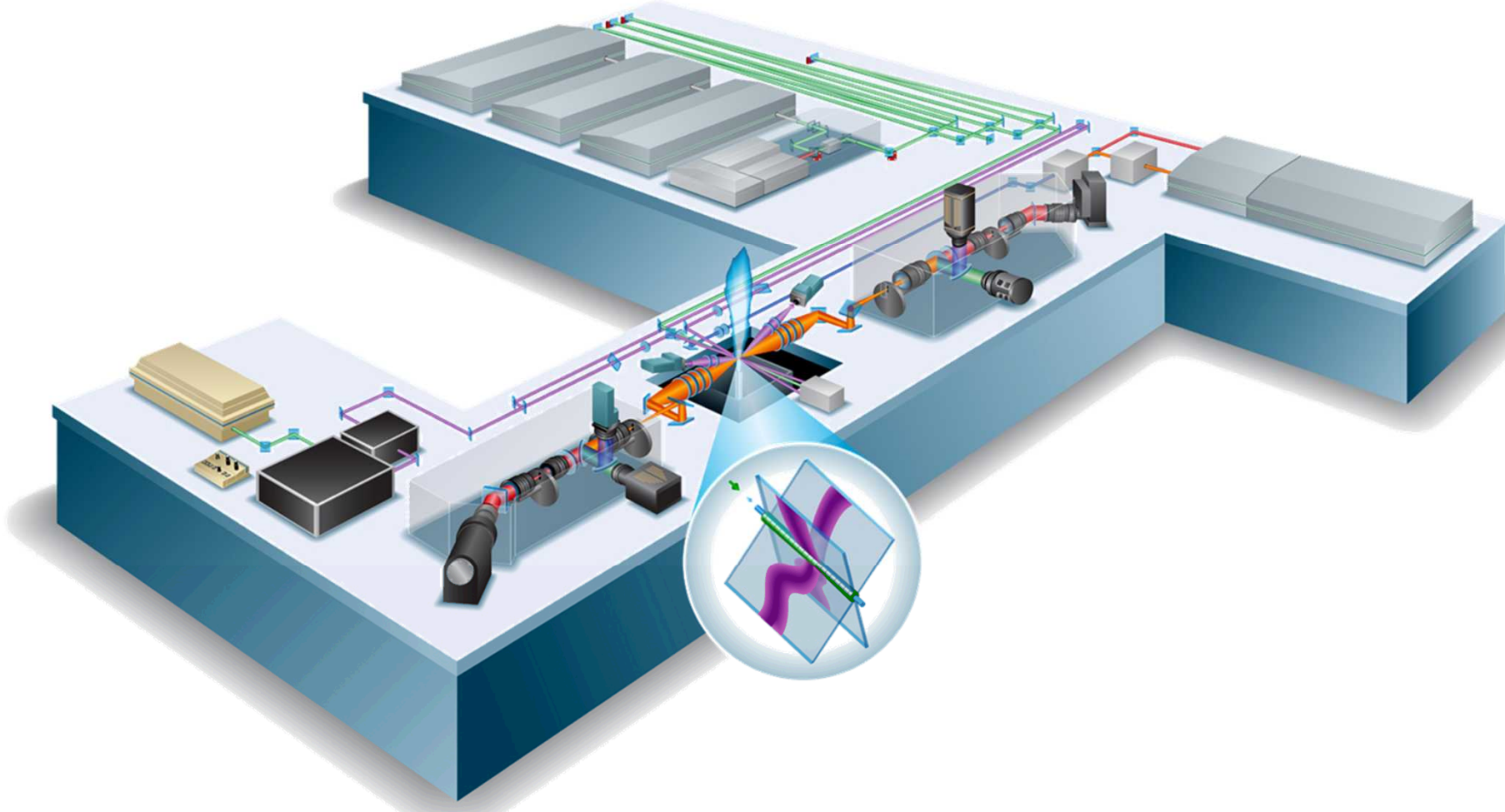
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Introduction

In combustion theory and modeling, turbulent flames are commonly classified as being either globally premixed or non-premixed. However, practical combustion systems can exhibit local flame regimes that do not fall into these idealized classifications. Variation in fuel-air mixing leads to partially premixed flames that can have local characteristics of both premixed and non-premixed flames. The goal of this work is to better understand the local structure of partially premixed methane flames by extracting additional information from Raman/Rayleigh measurements of temperature and major species. Data from a mildly turbulent lifted flame are analyzed using recently-developed methods that allow local reaction zones to be identified as premixed or non-premixed. Results provide new insight on the relative importance of local reaction zones as the overall flame structure evolves.

Experimental Approach

- Line-imaged Raman/Rayleigh/CO-LIF of major species and temperature
 - Four Nd:YAG lasers (532 nm, 1.0 J/pulse, ~400 ns)
 - Rotating shutter for Raman (21000 rpm, 3.9 μs gate)
 - Holographic grating, low-noise CCD (-110 C)
 - 230.1 nm two photon excitation of CO
- Wavelet adaptive thresholding and reconstruction (WATR) for denoising of all raw signals
 - 20 μm data spacing, ~50 μm effective resolution
 - Increased SNR on all scalars vs. 100 μm measurements
- Hybrid matrix inversion method with temperature dependent terms based on theoretical spectra from Ramses code (TU Darmstadt/h_da)



| Scalar | Precision, σ | Accuracy | Premixed flame |
|------------------|--------------|----------|----------------------|
| T | 0.7% | 2% | φ = 0.97, T = 2185 K |
| N ₂ | 0.6% | 2% | φ = 0.97, T = 2185 K |
| CO ₂ | 2.5% | 4% | φ = 0.97, T = 2185 K |
| H ₂ O | 1.7% | 3% | φ = 0.97, T = 2185 K |
| φ, ξ | 2.0% | 5% | φ = 0.97, T = 2185 K |
| CO | 3.3% | 10% | φ = 1.28, T = 2045 K |
| H ₂ | 5.5% | 10% | φ = 1.28, T = 2045 K |
| CH ₄ | 0.6% | 2% | φ = 1.28, T = 294 K |
| O ₂ | 0.7% | 3% | φ = 1.28, T = 294 K |

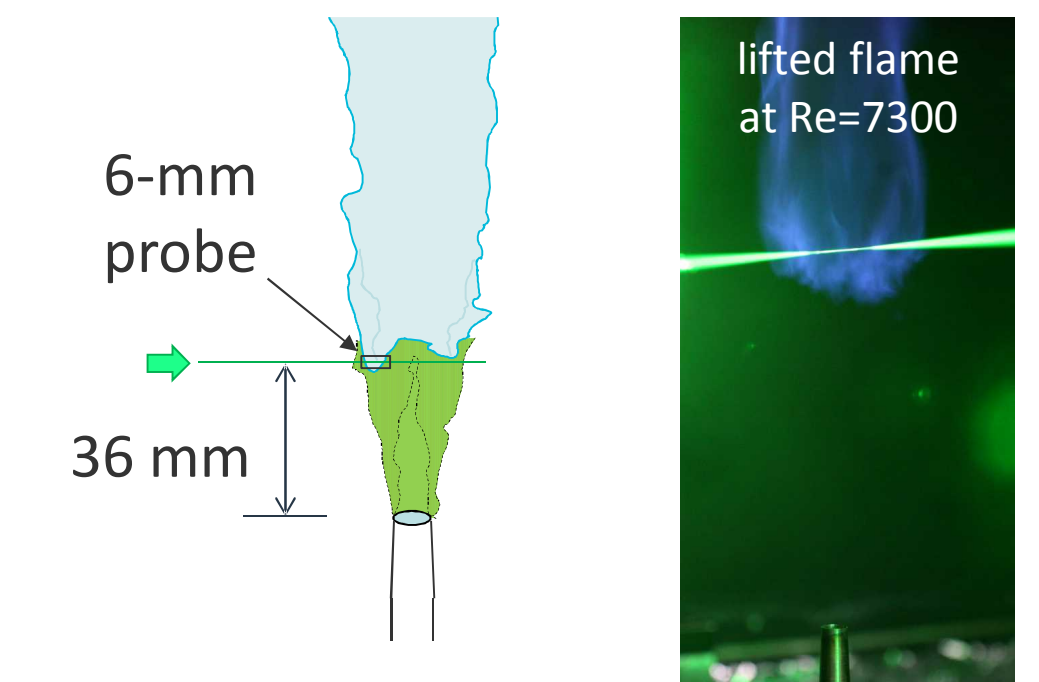
Laminar counterflow flames

- Horizontal counterflow burner with laser windows at each end
- Nozzle diameter = 11.1 mm, nozzle separation = 13 mm, annular N₂ flows
- Stable at intermediate strain rates
- Complete flame structure within 6-mm probe length (single-shot profiles)
- Three partially-premixed flames selected for comparison with counterflow flame simulations at match conditions
- PP1 has both inlets within flammability limits
- PP2 has both inlets outside flammability limits
- PP3 has fuel-side φ = 4.8, matching 2:1 air/CH₄ ratio of Sydney piloted flames

| | Inlet 1 | | Inlet 2 | | a (1/s) |
|------|----------------|----------------------|----------------|----------------------|---------|
| | φ ₁ | u ₁ (m/s) | φ ₂ | u ₂ (m/s) | |
| PP 1 | 0.7 | 0.29 | 1.4 | 0.39 | 114 |
| PP 2 | 0.4 | 0.22 | 1.8 | 0.16 | 60 |
| PP 3 | 0 | 0.31 | 4.8 | 0.3 | 101 |

Mildly turbulent lifted flame

- 8-mm jet diameter
- 0.3 m/s laminar coflow
- Jet exit Reynolds number = 2000



Gradient Free Regime Identification (GFRI)

- The GFRI method¹ allows local combustion regimes to be identified based on Raman/Rayleigh measurements, without requiring 3D gradient information.
- Starting from just temperature and major species, a constrained homogeneous reactor calculation (constant T,P) is applied to approximate the full thermochemical state for each instantaneous sample along the 6-mm line.
- Two key flame markers are calculated from the approximate full state:
 - Chemical mode: $CM := \text{sign}(\text{Re}(\lambda_e)) \times \log_{10}(1 + |\text{Re}(\lambda_e)|)$
 - Heat release rate: $HRR = \frac{-1}{\rho} \sum_{i \in N_s} \dot{\omega}_i h_{f,i}$
- Chemical explosive mode analysis² was developed as a technique for analyzing direct numerical simulations of turbulent flames.
- A CM zero crossing is an indicator of a premixed reaction zone (or auto-ignition).
- Mixture fraction (ξ; Bilger formulation; 0-air, 1-fuel) is a third flame marker.
- Criteria for detecting and characterizing local reaction zones, based on CM, HRR, and ξ, were developed using numerical test cases.¹

Premixed (P)

CM zero crossing and HRR peak near CM zero crossing

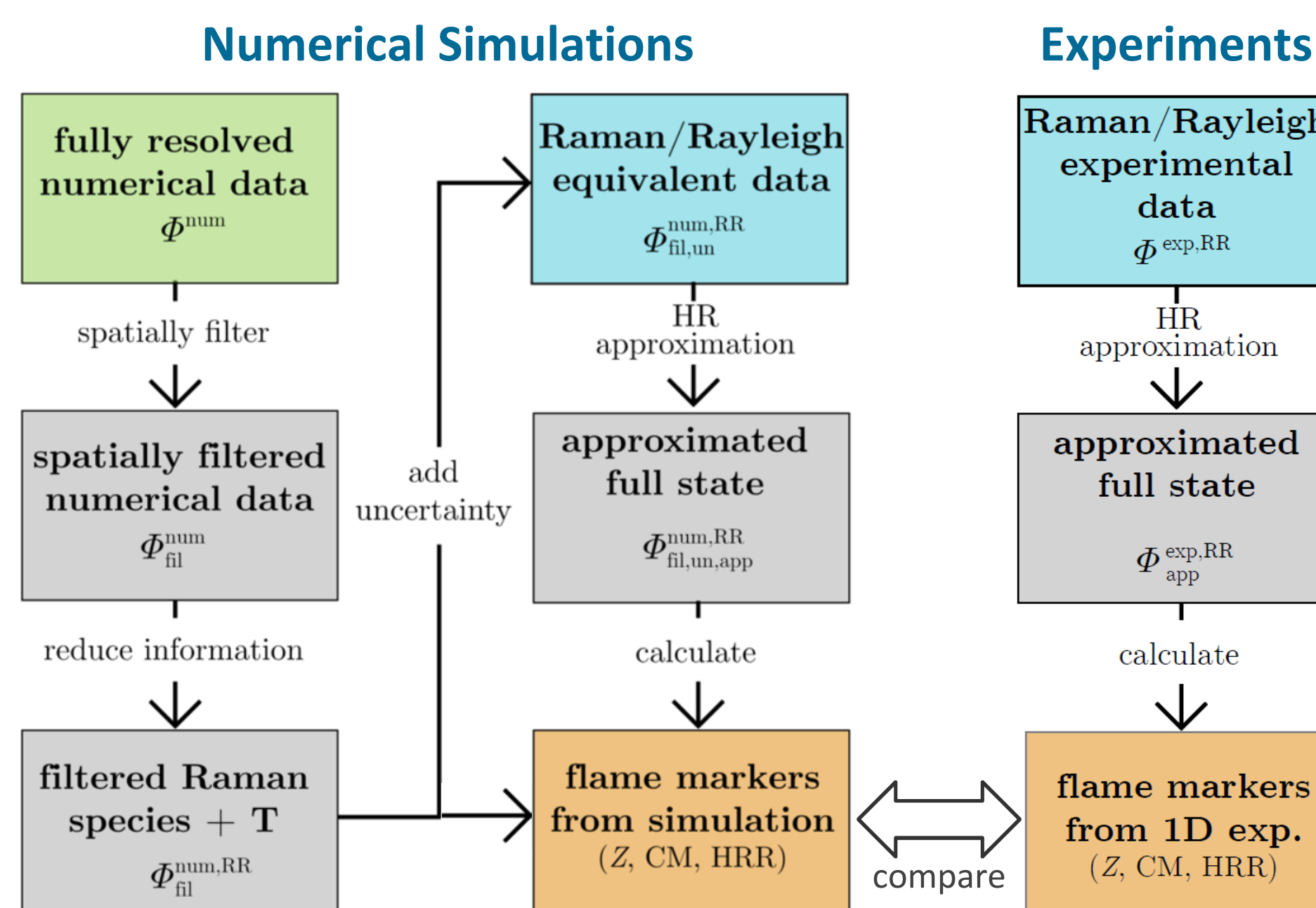
Non-premixed (NP)

negative CM values and significant HRR near ξ_{st}

1. S. Hartl, D. Geyer, A. Dreizler, G. Magnotti, R. S. Barlow, C. Hasse, Regime identification from Raman/Rayleigh line measurements in partially premixed flames (2017 submitted)
 2. T.F. Lu, C.S. Yoo, J.H. Chen, C.K. Law, Three-dimensional direct numerical simulation of a turbulent lifted hydrogen jet flame in heated coflow: a chemical explosive mode analysis, Journal of Fluid Mechanics 652 (2010) 45-64.

Constrained homogeneous reactor (HR) model:

- Fixed P and T (measured values)
- Seven major species account for more than 99% of mass in CH₄ flames
- Allow radicals and intermediates to build up from major species
- Constrain major species to stay within estimated experimental uncertainty intervals; this limits total time for reaction before CM and HRR are calculated



$$\Phi^{RR} = [T, Y_{CH_4}, Y_{CO_2}, Y_{H_2O}, Y_{CO}, Y_{H_2}, Y_{O_2}, Y_{N_2}]$$

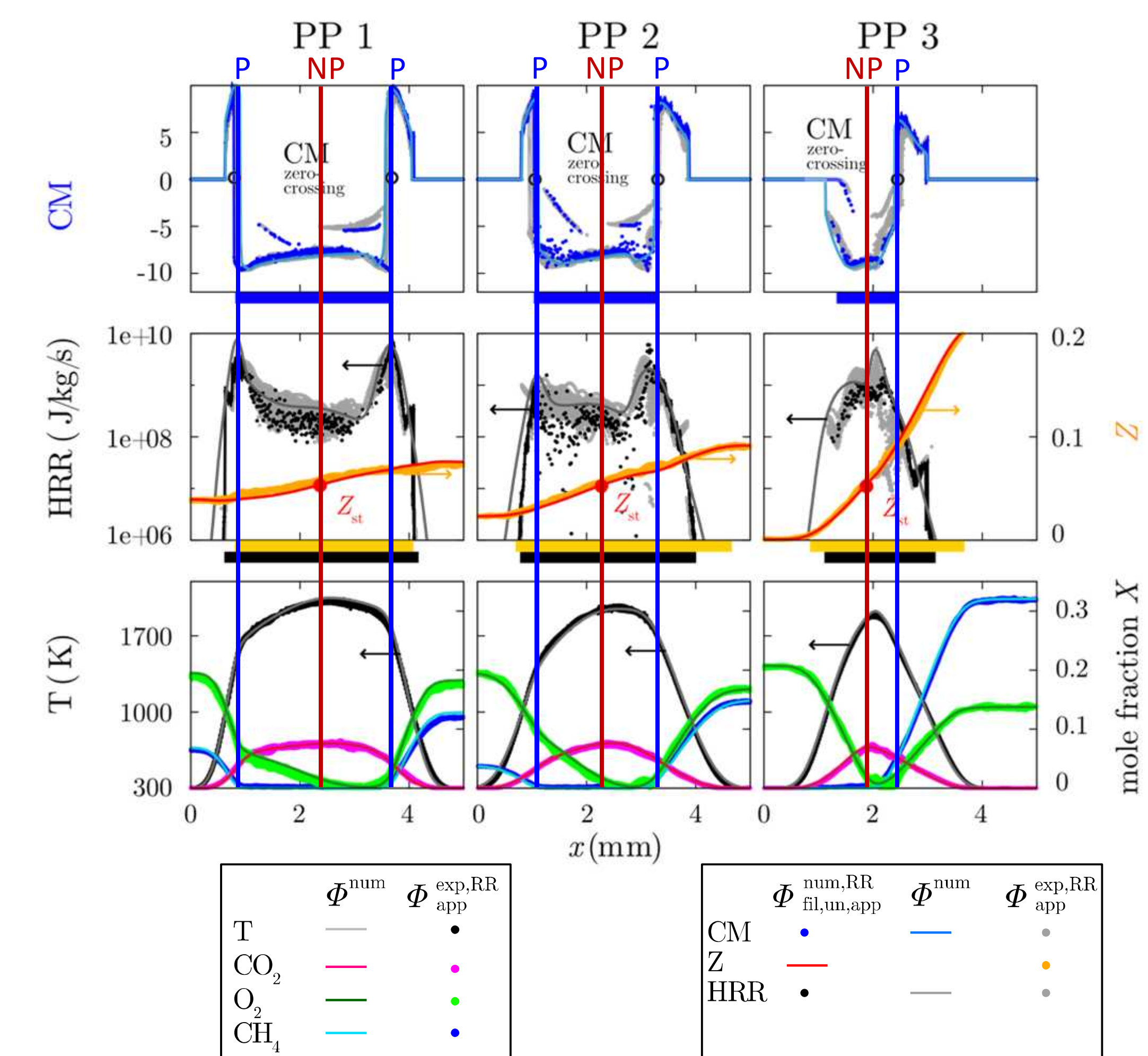


Fig. 1 Comparison of experimentally and numerically derived flame markers in counterflow flames.¹ Each experimental profile includes scatter data from 50 laser shots (12500 data points).

Lifted Flame Results and Discussion

- The lifted methane flame shows a range of instantaneous structures from flames that are dominantly premixed in character to flames that are dominantly non-premixed.
- Differences are seen in the magnitude of the CM zero crossing (ΔCM) and the location of the maximum HRR relative to the CM zero crossing.
- In near-stoichiometric premixed flame reaction zones the CM value changes by ~20 at the zero crossing, and the maximum HRR occurs at the same position as the CM zero crossing, as shown below in Fig. 2a.
- As the CM zero crossing moves to richer conditions (Fig. 2b,c) the heat release rate at the CM crossing becomes less significant and ΔCM decreases (see Fig. 3).
- The minimum value in the CM profile occurs at the point of maximum HRR in all examples.

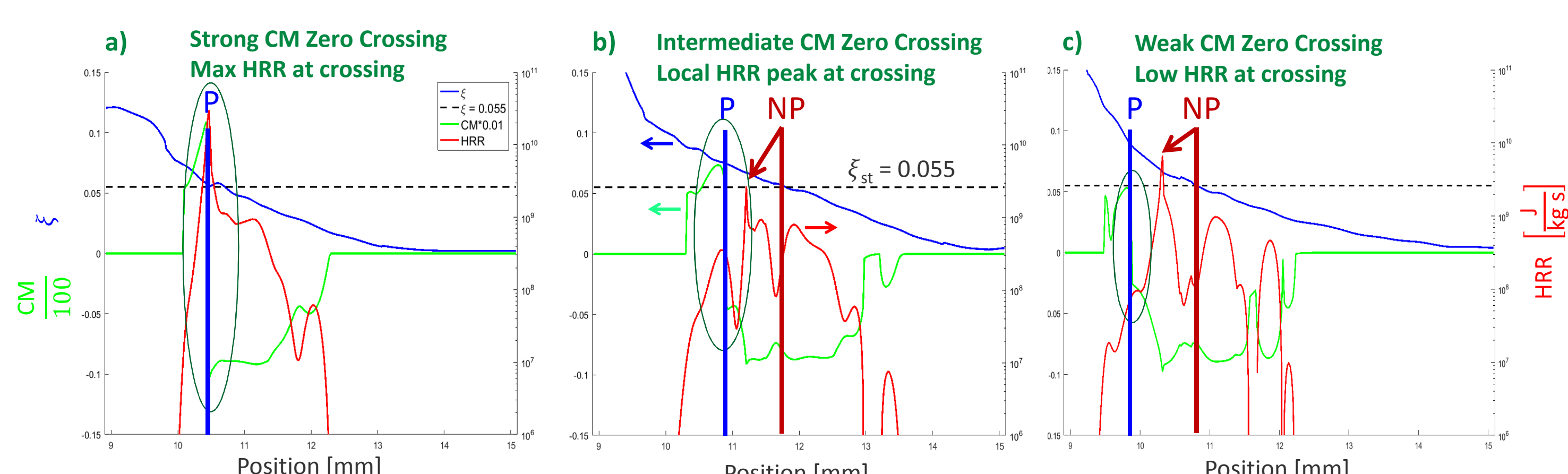


Fig. 2 Instantaneous profiles of the three GFRI flame markers, illustrating the evolution from premixed toward non-premixed structure

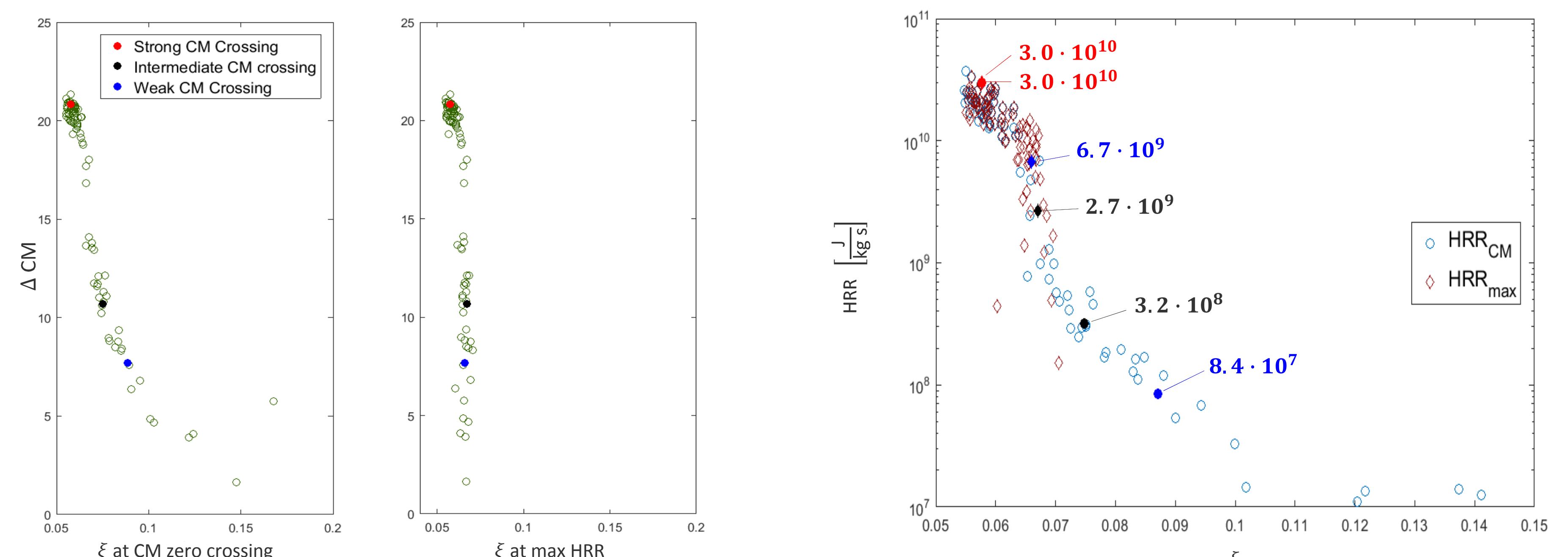


Fig. 3 ΔCM and HRR plotted vs. the corresponding ξ value for 92 instantaneous realizations in the lifted flame. Examples from Figure 2 are marked by solid symbols.

Considering only CM zero crossings at stoichiometric and rich conditions, the following observations are made:

- Dominantly premixed reaction zones have CM crossings and maximum HRR close to stoichiometric conditions.
- As the CM zero crossing moves to richer conditions, the strength (ΔCM) decreases
- For CM crossings with ξ ≥ 0.07 the HRR at the crossing becomes very low and the maximum HRR location moves back toward ξ ~ 0.065, where CM is strongly negative, indicating an overall flame structure that is dominantly non-premixed.
- While there is significant uncertainty in HRR derived from the experiments, the qualitative trend relating HRR at the CM crossing to ξ at the CM crossing is consistent across three orders of magnitude in local heat release rate.

Work in Progress: Parametric numerical study of laminar counterflow flames; Investigation using CSP methods to monitor the HR; Application of GFRI to data from the Sydney piloted inhomogeneous flames; Add quantitative OH.