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Experimental Insights on Multi-Mode Combustion

Robert Barlow

Sandia National Laboratories

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Collaborators

- Dr. Sandra Hartl (GFRI analysis)
- David Butz (experiments on TUD burner)
- Prof. Dirk Geyer
- Prof. Christian Hasse
- Prof. Andreas Dreizler

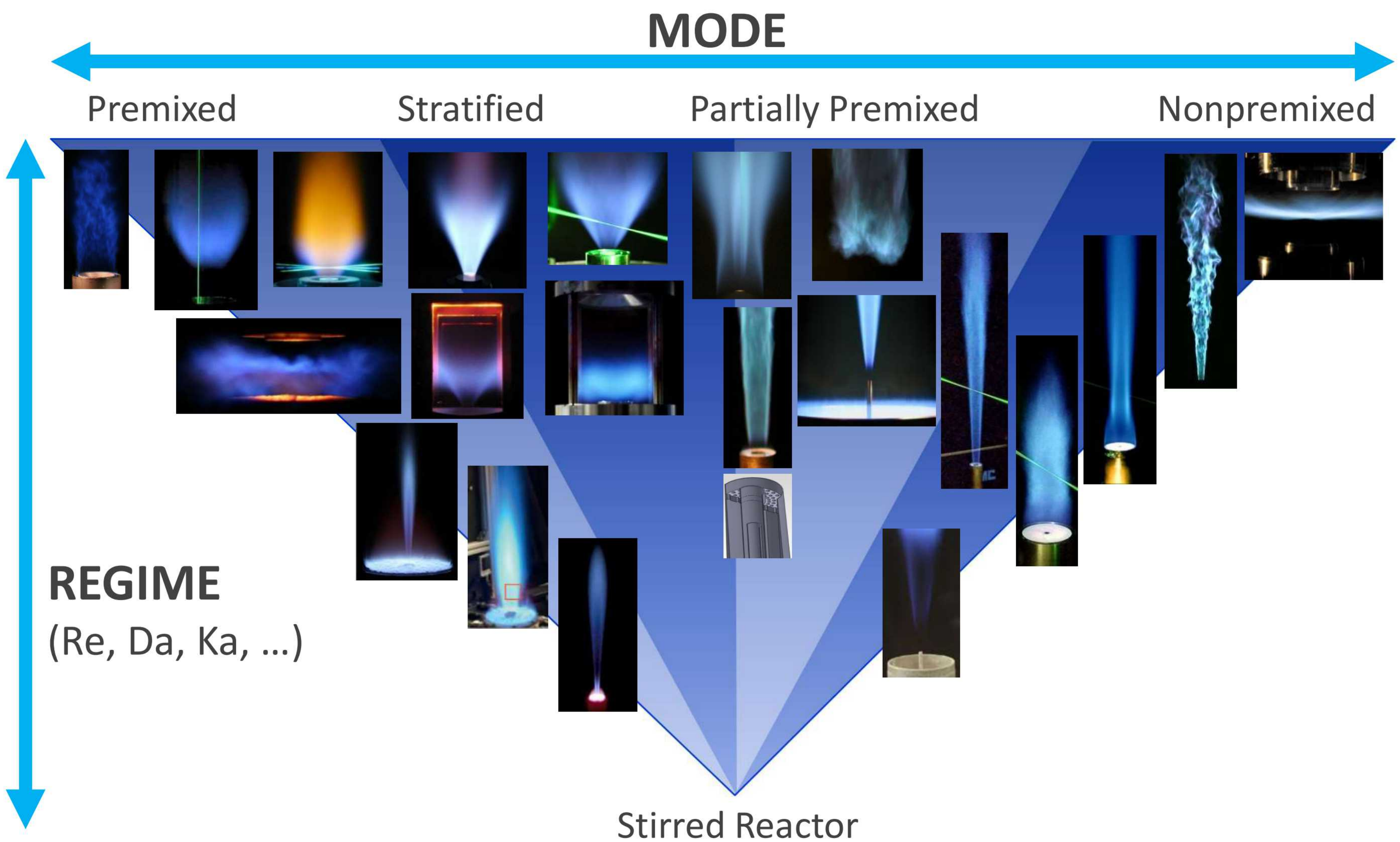
- Sean Meares (experiments on Sydney burner)
- Hugh Cutcher (experiments on Sydney burner)
- Dr. Matthew Dunn
- Prof. Assaad Masri

- Support for experiments at Sandia was provided by the US Department of Energy, Office of Basic Energy Sciences

Outline

- Background on partially premixed flames and multi-mode combustion
- Gradient free regime identification (GFRI)
  - Motivation
  - Definitions
  - Review of applications to laminar flames and lifted turbulent methane flame
- Two multi-mode burners (TU Darmstadt and Sydney University)
- Experimental apparatus (Sandia)
- Automated characterization of turbulent reaction zones from Raman/Rayleigh/CO-LIF data
- Conclusions and outlook

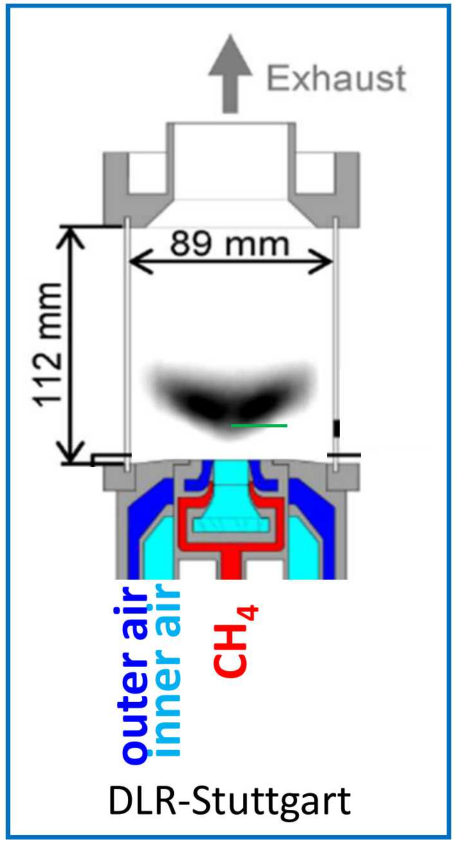
Combustion modes and regimes

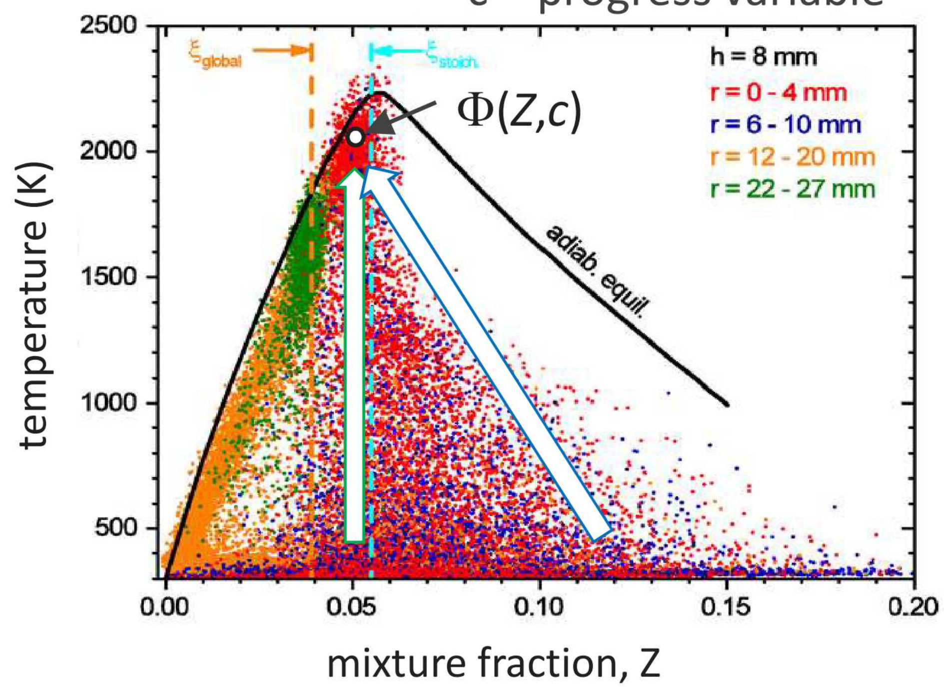


- Interactions of turbulence, molecular transport, and chemistry are expressed differently in the different combustion modes and regimes
- Partially premixed flames can combine multiple types of reaction zones within the same overall flame structure
- Multi-mode combustion is not well understood at a fundamental level
- Challenging for models
- Topic for TNF workshop

Mixed mode combustion is common in practical systems

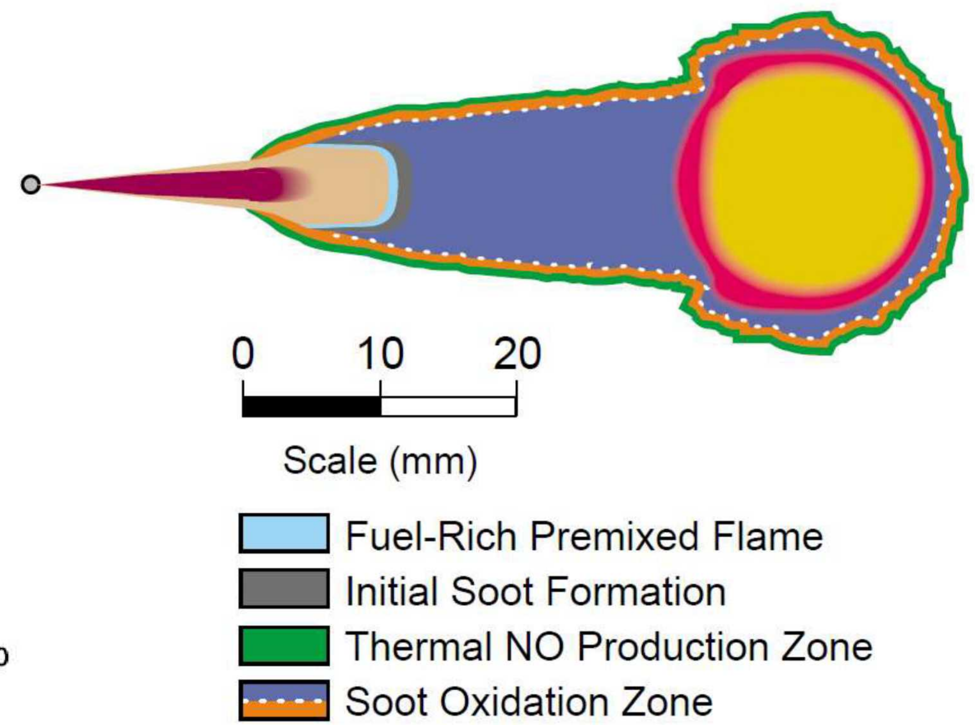
Gas turbine combustion





- Meier et al., Experimental Thermal and Fluid Science 73 (2016) 71–78

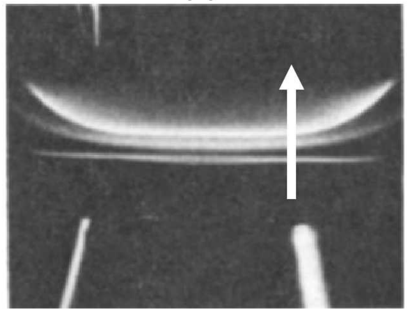
Diesel engine combustion



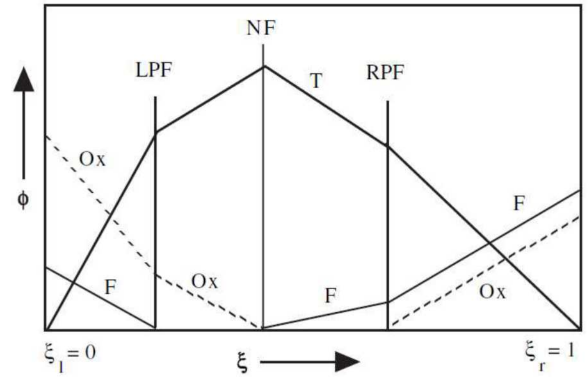
- Dec 1997 SAE paper 970873 DOI: https://doi.org/10.4271/970873

Partially Premixed Combustion

Laminar Opposed Flow

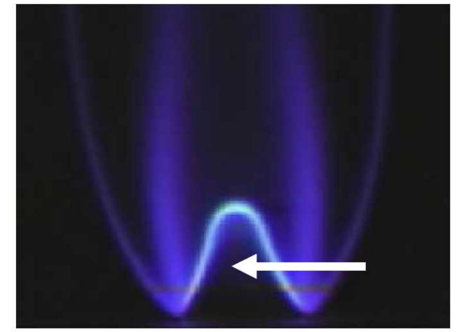


Sohrab et al. PCI 1984



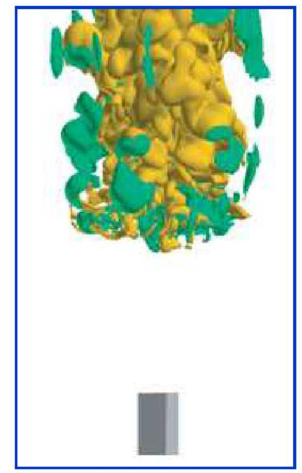
S.K. Aggarwal, PECS 35 (2009) 528–570

Laminar Edge (Triple) Flame

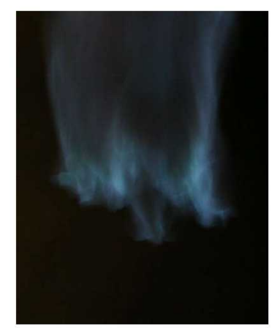


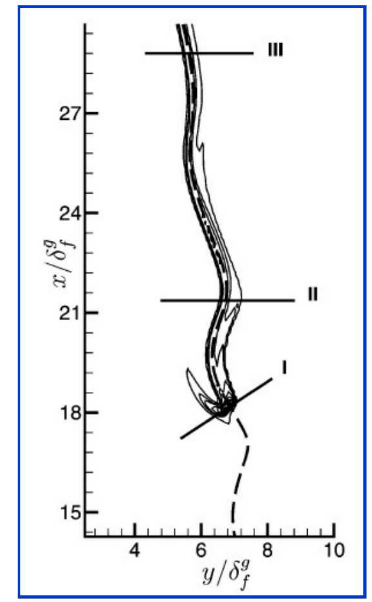
S.K. Aggarwal, PECS 35 (2009) 528–570

- Takeno Flame Index (Yamashita, PCI 1996): $\nabla Y_F \cdot \nabla Y_O$
  - Identify premixed/nonpremixed flame structures in lifted H_2 jet flame DNS (Mizobuchi et al. PCI 2002)
  - Normalized flame index: $(\nabla Y_F \cdot \nabla Y_O)/|\nabla Y_F \cdot \nabla Y_O|$
    +1 for premixed, -1 for nonpremixed.
    Still used, but overly simplistic and potentially misleading
  - Good discussion in: Domingo et al. (CNF 2005), Fiorina et al. (CNF 2005), Knudsen & Pitsch (CNF 2009)
- Full spectrum of flame structures between premixed and non-premixed



Lifted H_2 flame DNS





Lifted HC flame DNS

Gradient-free regime identification (GFRI)

Regime (mode) identification from Raman/Rayleigh line measurements in partially premixed flames

Hypotheses:

1. Major species and temperature from experiments are a footprint of thermochemical state of each sample
2. The full thermochemical state can be approximated by a constrained homogeneous (0D) reactor calculation
3. Relevant flame markers (heat release rate and chemical explosive mode) can be calculated from this approximated state
4. Combinations of flame markers can reliably detect and characterize reaction zones

Experiment

Approximation

Flame markers

Identification

Hartl et al., Combust. Flame 189, 2018; Hartl et al., Proc. Combust. Inst. 37, 2019

GFRI – Flame markers

Bilger mixture fraction (element based) [1]:

(characterizing non-homogeneous systems)

$$Z = \frac{\frac{2(Y_C - Y_{C,ox})}{W_C} + \frac{Y_H - Y_{H,ox}}{2W_H} - \frac{Y_O - Y_{O,ox}}{W_O}}{\frac{2(Y_{C,fuel} - Y_{C,ox})}{W_C} + \frac{Y_{H,fuel} - Y_{H,ox}}{2W_H} - \frac{Y_{O,fuel} - Y_{O,ox}}{W_O}}$$

Chemical explosion mode analysis [2,3]:

(zero-crossing identifies premixed reaction zones, ignition and extinction processes)

- Evaluate the eigenvalues of the chemical Jacobian
- Eigenvalue with max. real part is defined as λ_e

$$\mathrm{CM} = \mathrm{sign}(\mathrm{Re}(\lambda_e)) \times \log_{10}(1 + |\mathrm{Re}(\lambda_e)|)$$

Heat release rate [4]:

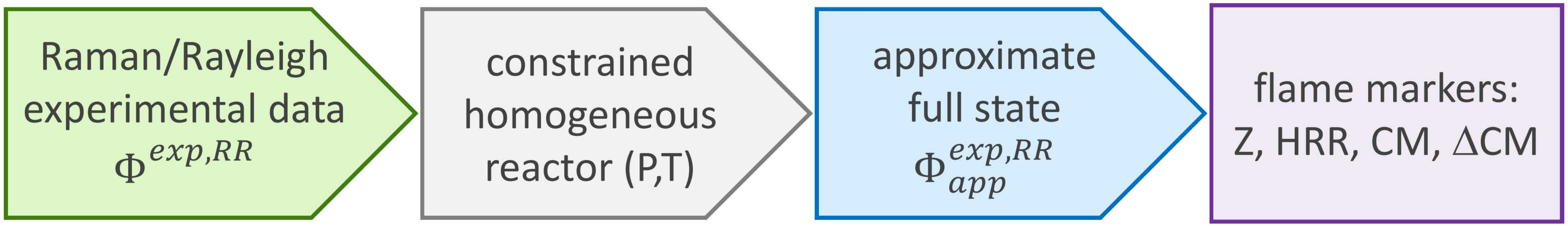
(use local value to detect reaction zones)

$$\mathrm{HRR} = -\,1/\rho \sum_{I \in N} \dot{\omega}_I h_{f,i}$$

[1] R.W. Bilger et al., Combust. Flame 80 (1990) *[2] T.F. Lu et al., J. Fluid Mech. 652 (2010)* *[3] R. Shan et al., Combust. Flame 159 (2012)* *[4] P. Domingo et al., Combust. Flame 140 (2005)*

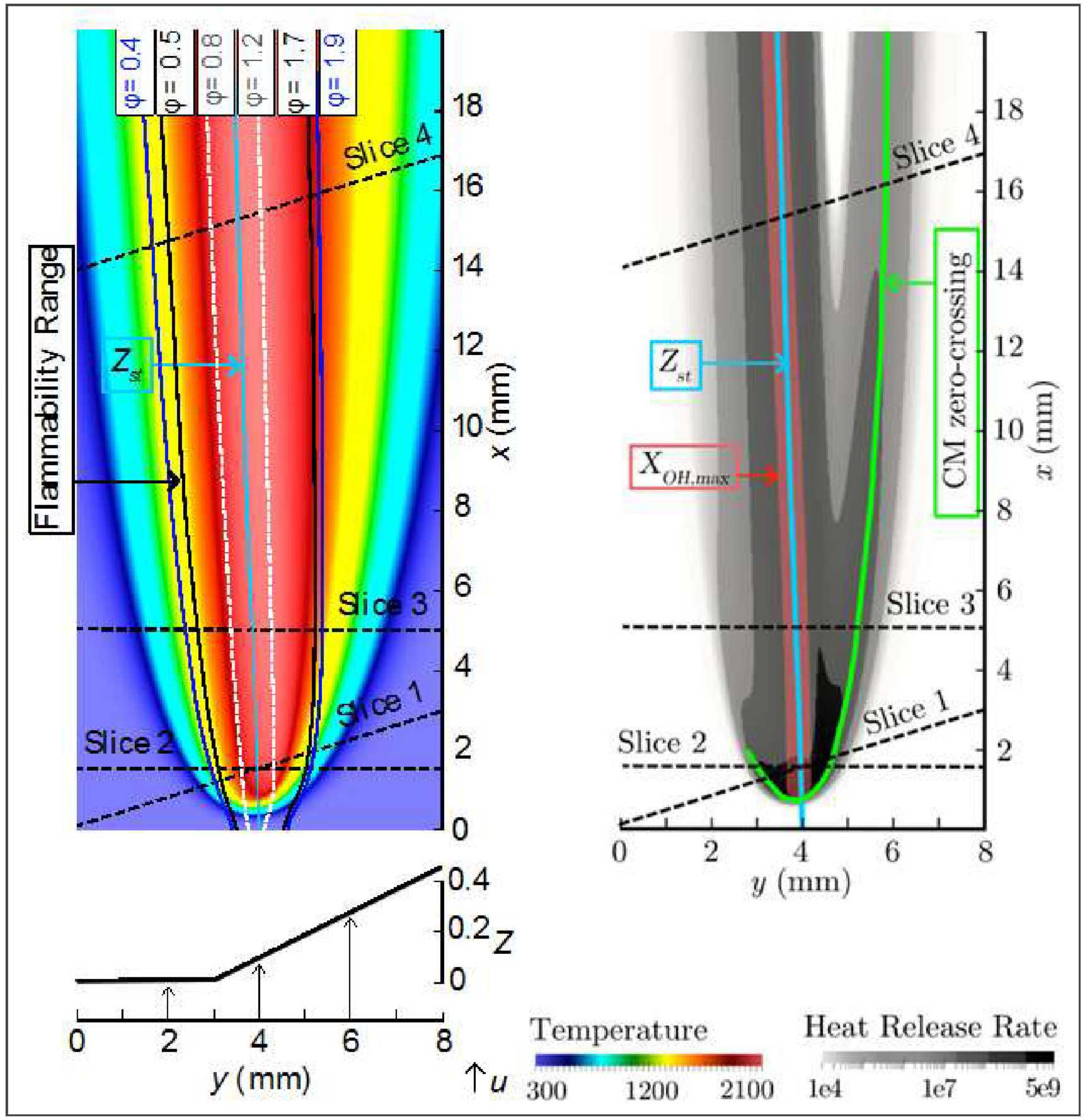
Procedure to approximate the full thermochemical state

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



- For methane flames, major species > 0.99 mass fraction
- 0D reactor: constant temperature, constant pressure, long residence time
- Allow minor species, radicals to build up from zero to steady state
- Calculate flame markers
- Original approach: Constrain major species to stay within experimental uncertainty
- Current approach: Constrain major species (except CH4) to initial values (best available information)
  Evaluate sensitivity to experimental uncertainty using UQ methods

Identification criteria developed using laminar flame simulations



- 1D CH_4/air counterflow flames:
  - Non-premixed
  - Premixed
  - Partially premixed
- 2D CH_4/air triple flame:
  - Lean and rich premixed branches
  - Trailing non-premixed flame
  - Four 1D slices
- Identification criteria

Premixed	**Non-Premixed**
• CM zero-crossing • HRR local max near crossing	• negative CM values • significant HRR near Z_{st}

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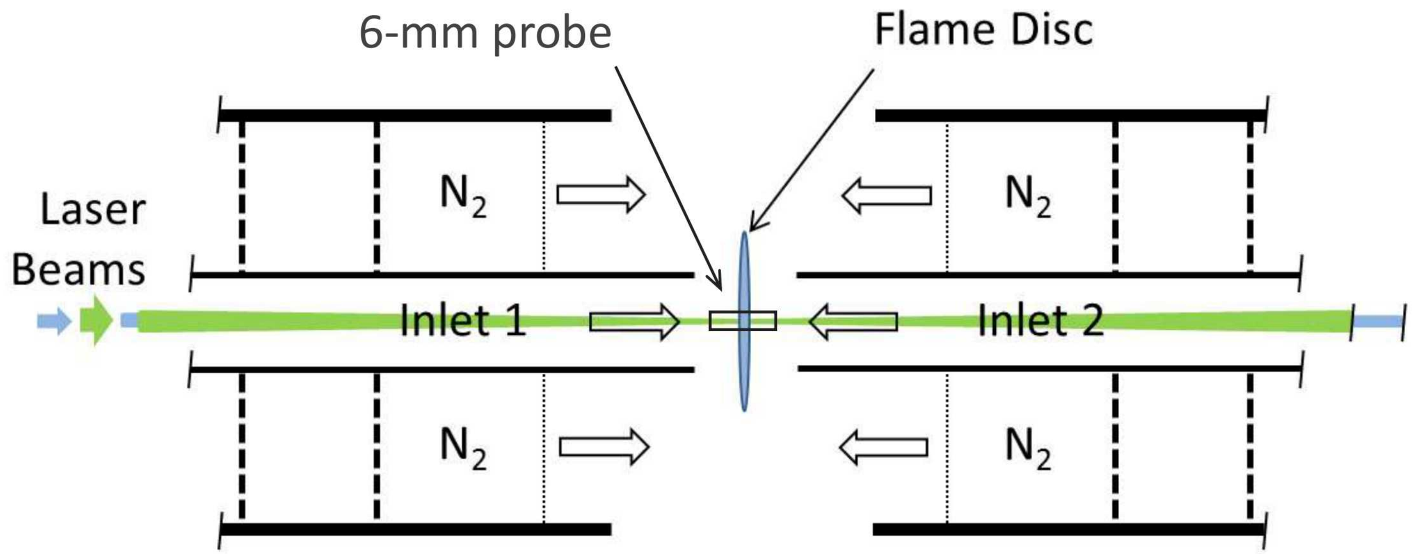
Hartl, Geyer, Dreizler, Magnotti, Barlow, Hasse (Combust. Flame, 189, 2018)

GFRI method validated using counterflow flame experiments



Three partially premixed flames

	Inlet 1		Inlet 2		
	φ_1	u (m/s)	φ_2	u (m/s)	*a (1/s)*
PP1	0.7	0.29	1.4	0.39	114
PP2	0.4	0.22	1.8	0.16	60
PP3	0	0.31	4.8	0.3	101

PP1 – both inlets flammable

PP2 – both inlets outside flammability limits

PP3 – fuel side matches Sydney piloted inhomogeneous jet flames

Hartl, Geyer, Dreizler, Magnotti, Barlow, Hasse (Combust. Flame, 189, 2018)

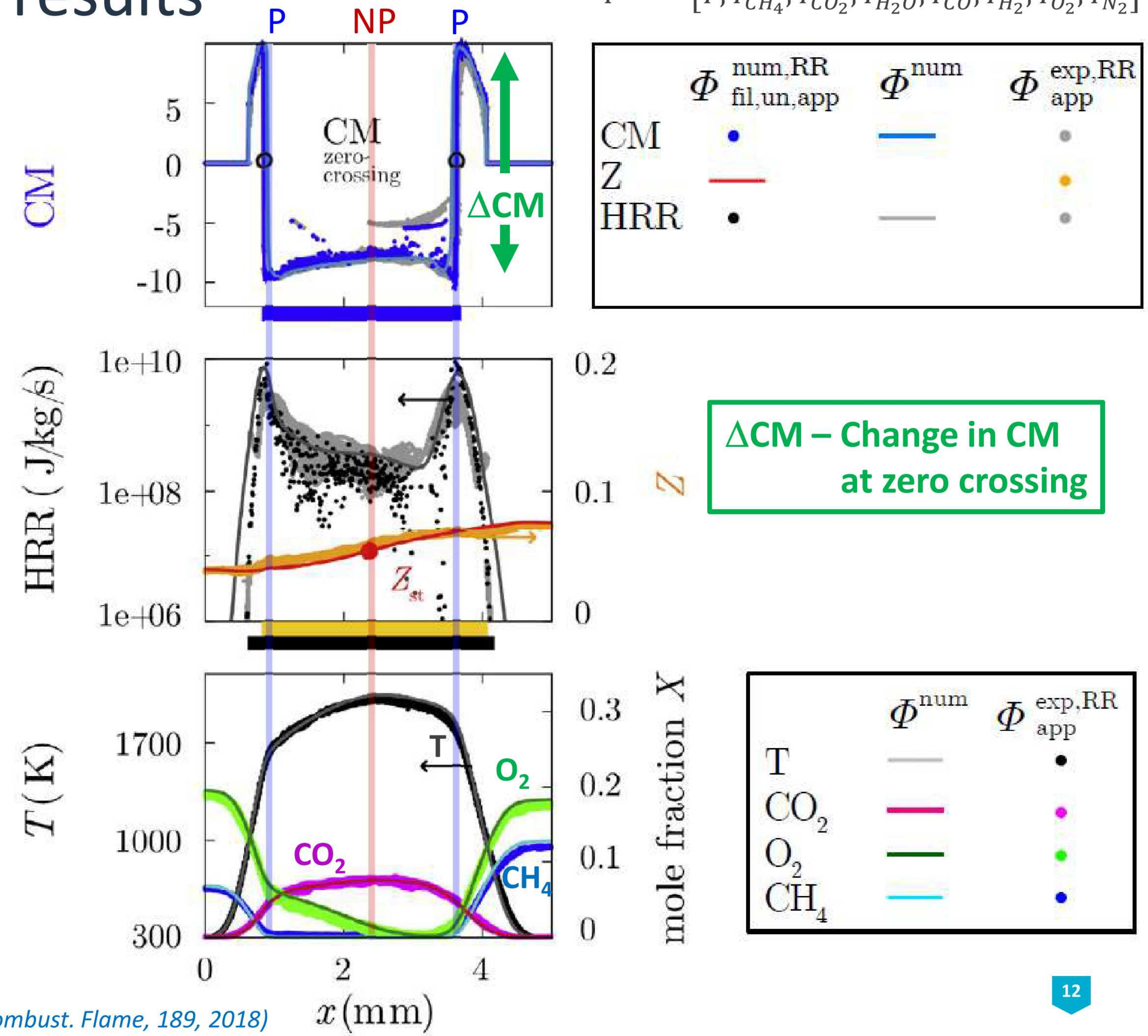
Laminar counterflow flame results

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

- Flame PP1: ϕ_1=0.7, ϕ_2=1.4
- CM
  - Approximation yields accurate zero crossings
  - Good agreement across most of the profile
- HRR
  - More sensitive to uncertainty
  - local peaks can still be identified

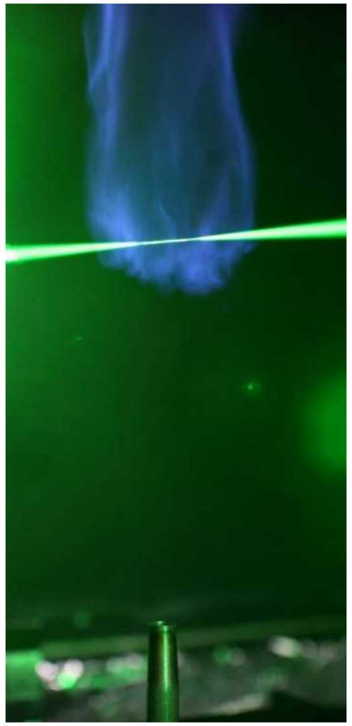
- **Flame markers and reaction zones are correctly identified from the Raman/Rayleigh data**

- **Relative strength of different reaction zones can be assessed**

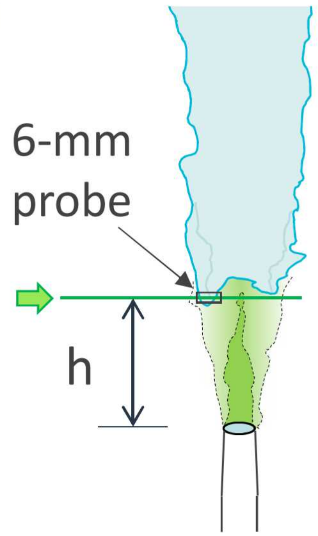


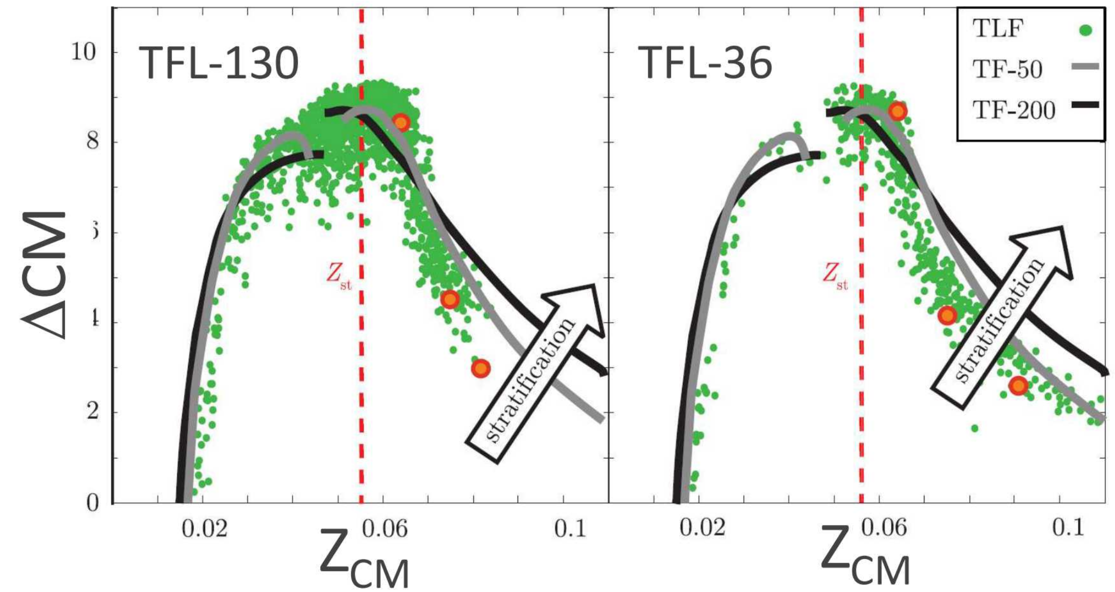
Hartl, Geyer, Dreizler, Magnotti, Barlow, Hasse (Combust. Flame, 189, 2018)

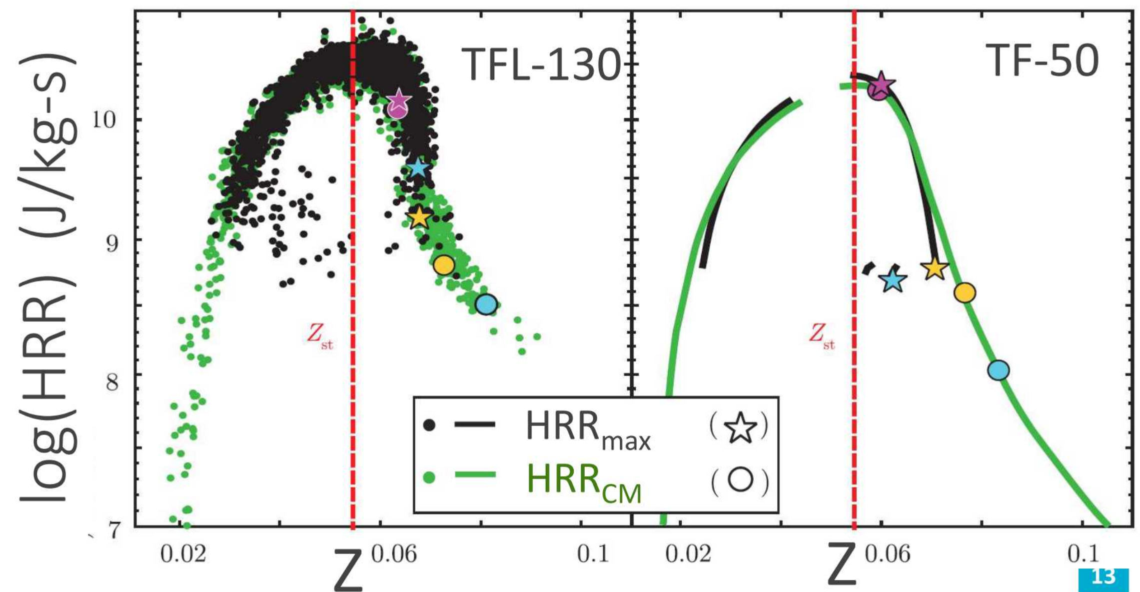
Lifted flames and the correlation of Z_{CM}, ΔCM, HRR



- Mildly turbulent lifted flames
  - D = 8.0 mm
  - 0.3 m/s coflow
  - Re_{jet} = 2000, 7330
  - liftoff heights: h/D = 4.5, 16





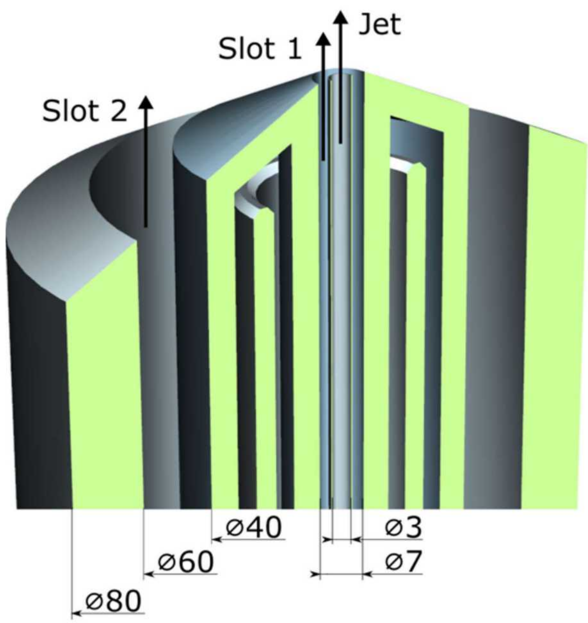


- **HRR and ΔCM decrease as Z_{CM} moves away from most reactive range**
- **HRR_{max} switches to non-premixed reaction zone as premixed zone weakens**
- **Similar in experiment and simulation**

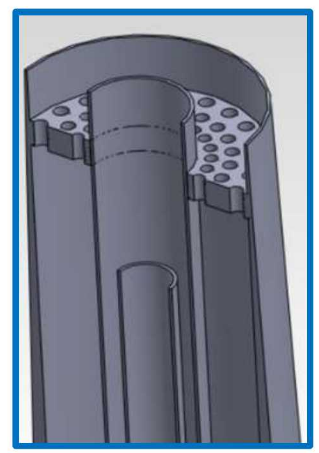
Hartl et al., Proc. Combust. Inst. 37, 2019

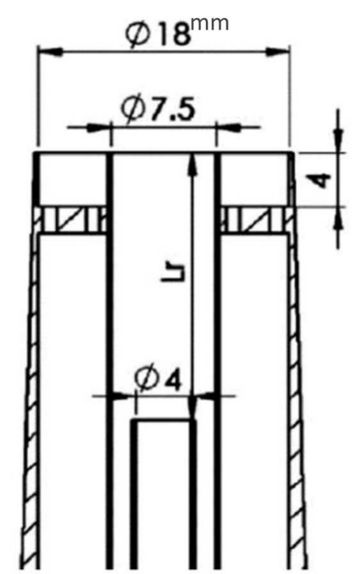
Two burners for investigation of multi-mode combustion

- TU Darmstadt Multi-Regime Burner (MRB)
  - Central jet: high-velocity CH_4/air (rich)
  - Annular slot 1: air flow
  - Annular slot 2: Lean CH_4/air (ϕ=0.8)
  - 1 m/s outer air coflow
- Outer premixed flame generates recirculation zone of hot products
- Variable mixing of jet, air, product flows below lifted inner reaction zone



- Sydney Univ. Piloted Inhomogeneous Jet Burner
  - Retractable central fuel tube (CH_4)
  - Annular air (overall air/CH_4 ratio = 2)
  - Variable mixing upstream of the jet exit plane
  - Stoichiometric annular pilot flame
- Enhanced stability with recess of Lr = 75mm
- Previous interpretation: Premixed combustion in the near field, followed by transition to non-premixed burning downstream





TU Darmstadt “Multi-Regime” Burner (MRB)

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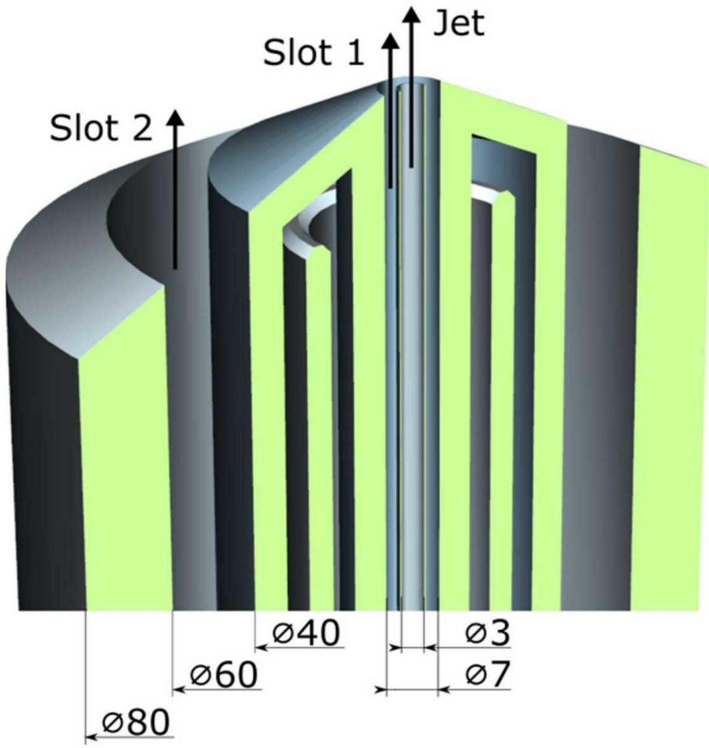
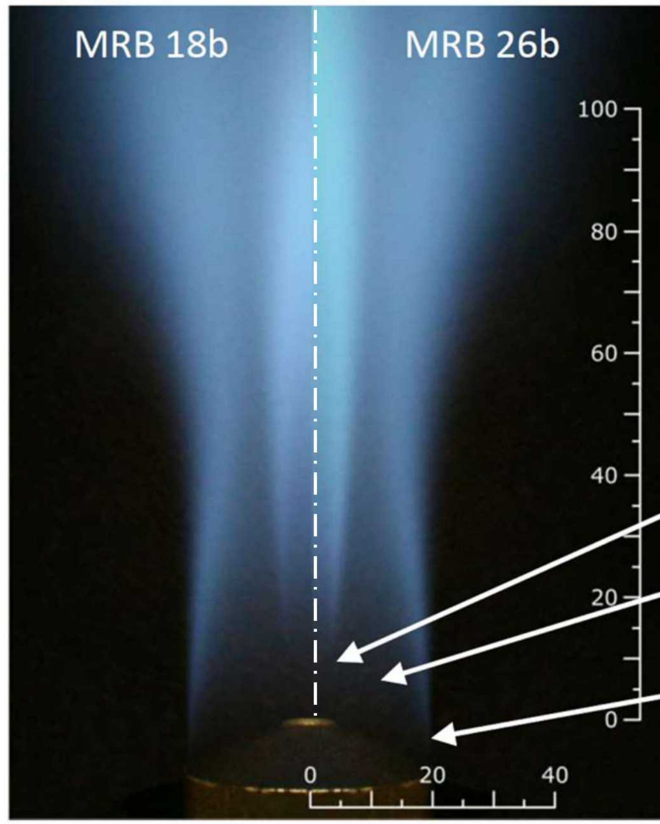
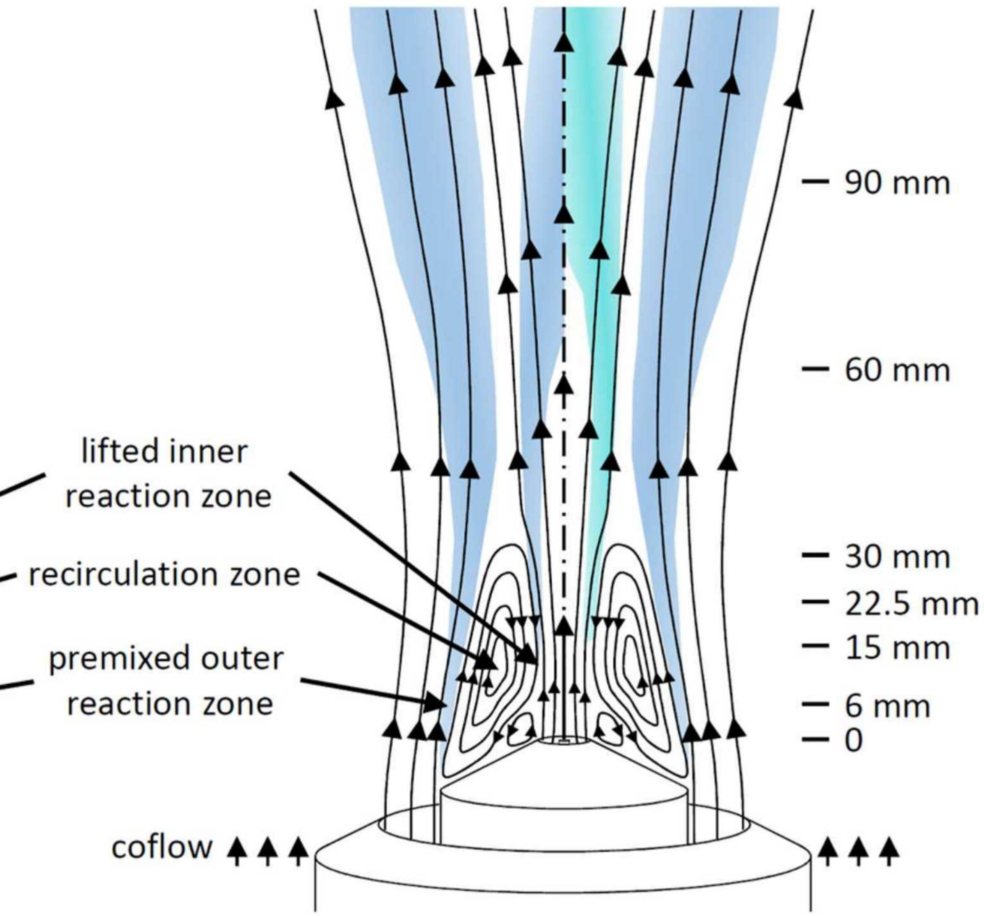


	jet		slot 1			slot 2	
	φ	u [m/s]	φ	u [m/s] a	u [m/s] b	φ	u [m/s]
MRB14	1.4	105	0	7.5	15	0.8	20
MRB18	1.8						
MRB22	2.2						
MRB26	2.6						





- Eight cases studied: Raman/Raleigh/LIF and PIV
- Focus on two cases: MRB18b, MRB26b

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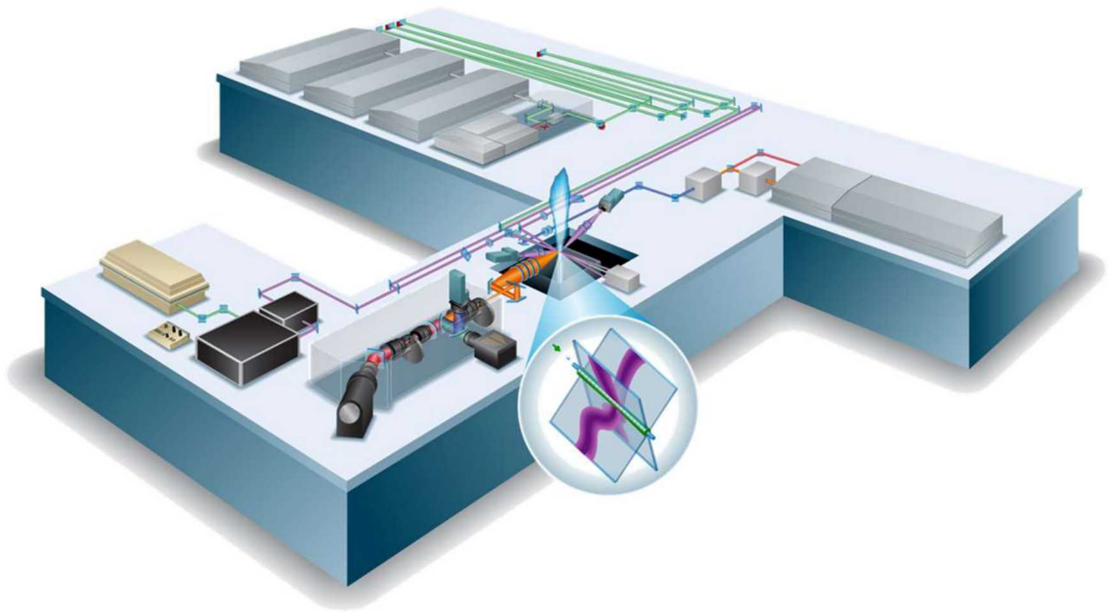


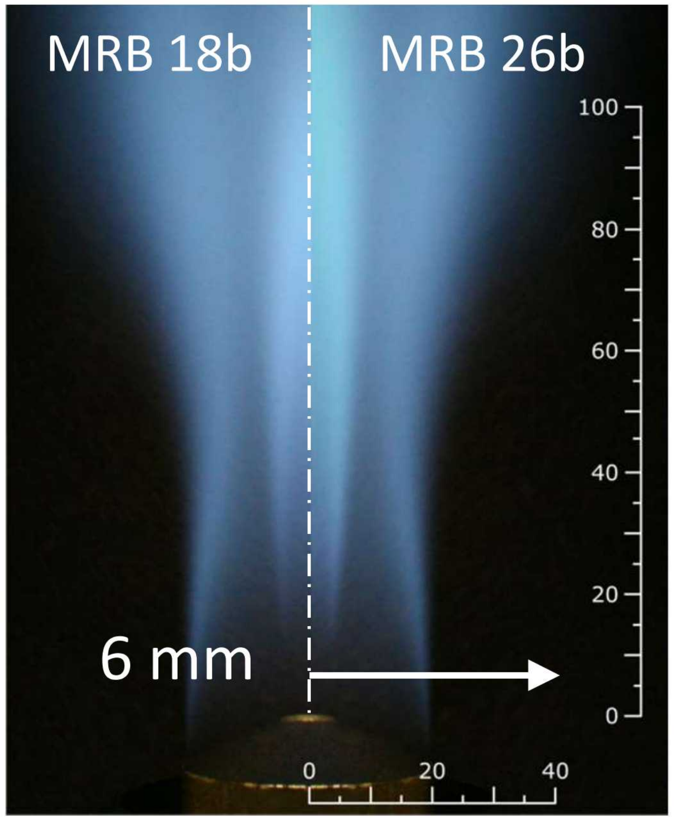
Scalar	Precision, σ	Accuracy	Premixed flame
T	0.7%	2%	$\phi = 0.97, T = 2185$
N_2	0.6%	2%	$\phi = 0.97, T = 2185$
CO_2	2.5%	4%	$\phi = 0.97, T = 2185$
H_2O	1.7%	3%	$\phi = 0.97, T = 2185$
ϕ, Z	2.0%	5%	$\phi = 0.97, T = 2185$
CO	3.3%	10%	$\phi = 1.28, T = 2045$
H_2	5.5%	10%	$\phi = 1.28, T = 2045$
CH_4	0.6%	2%	$\phi = 1.28, T = 294$
O_2	0.7%	3%	$\phi = 1.28, T = 294$

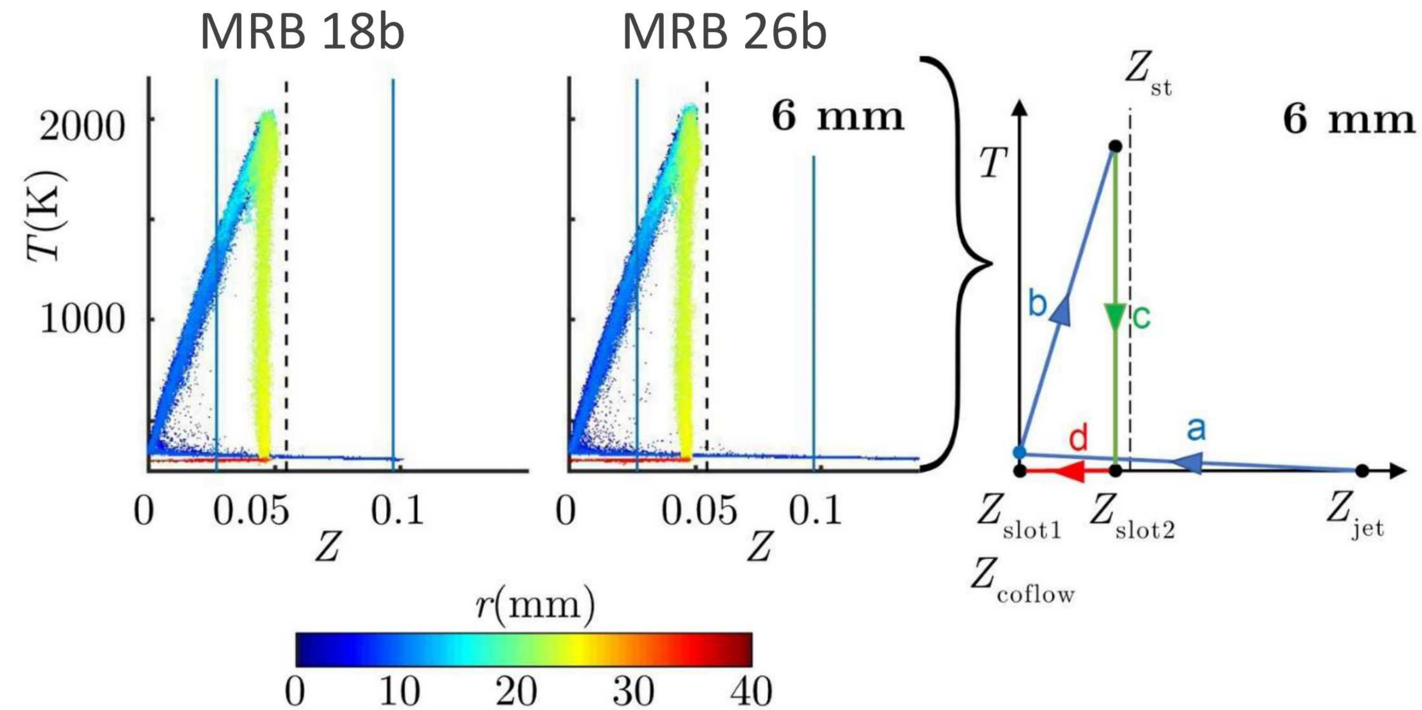
Table 2: Representative uncertainties in scalar measurements at flame conditions.

- **Raman/Rayleigh**
  - Four Nd:YAG lasers (1.0 J/pulse, ~400 ns)
  - Rotating shutter (21000 rpm, 3.9 μs gate)
  - Low-noise CCD (-110 C)
  - **6-mm probe length**
- **CO-LIF**
  - 230.1 nm excitation
  - Lower noise, less interference
- **Wavelet adaptive thresholding & reconstruction (WATR)**
  - **Reduced noise** in all signals
  - 20 μm data spacing, **50 μm resolution**
- Hybrid matrix inversion
  - Temperature dependent response based on theoretical Raman spectra

Temperature vs. mixture fraction

- The profile at 6 mm is below the inner flame stabilization zone

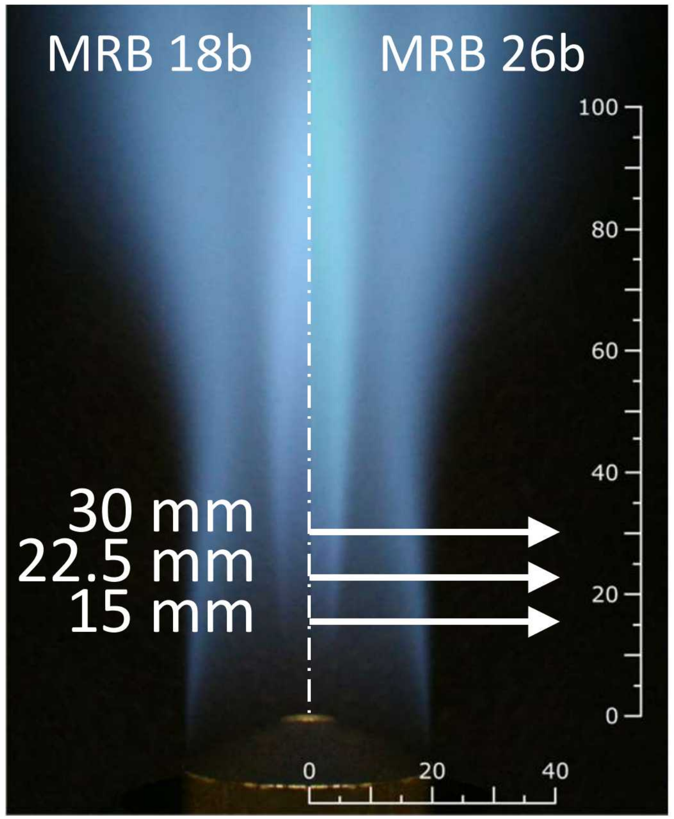




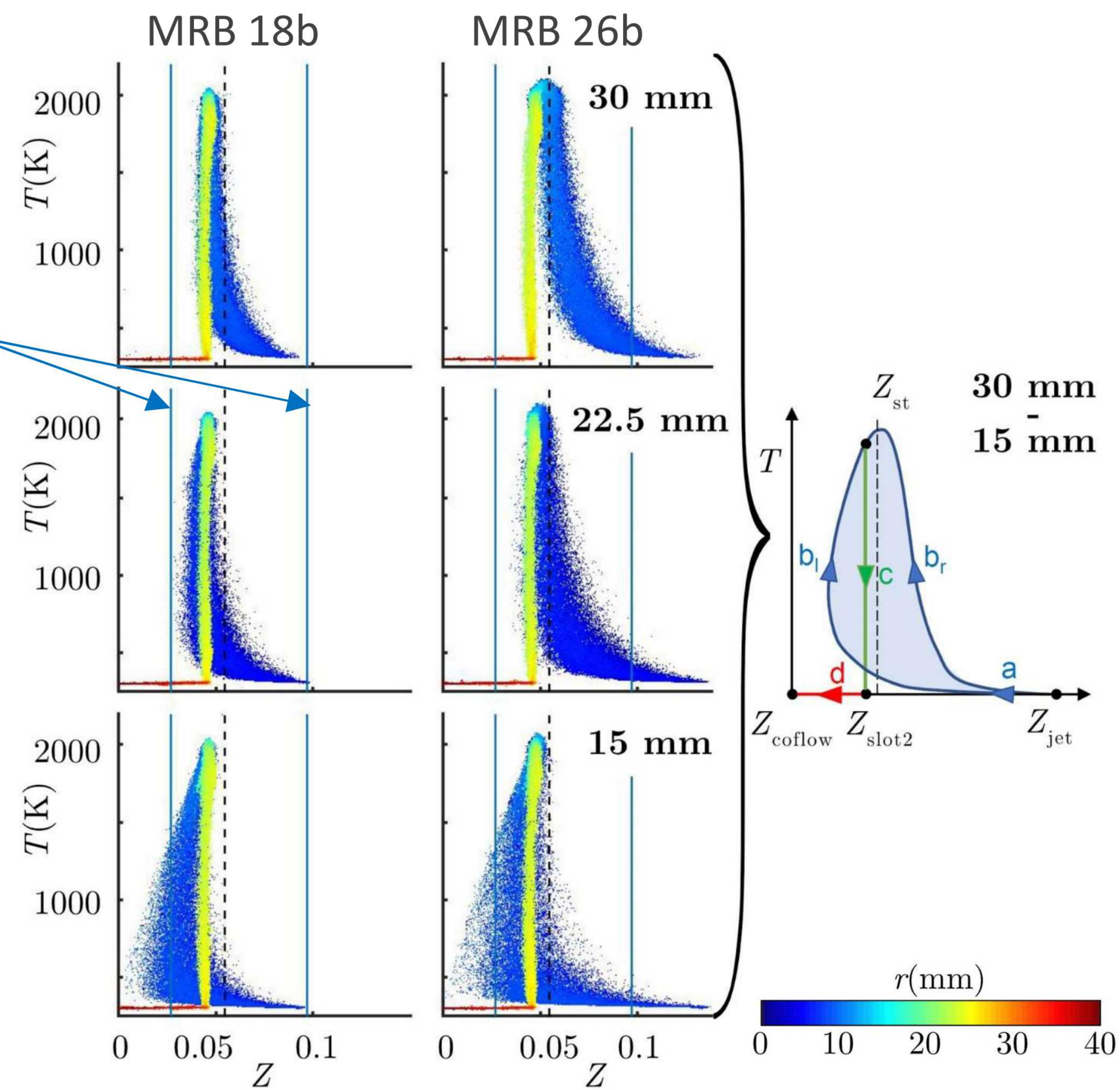
- Line a: mixing of jet fluid with slot 1 air (warm)
- Line b: mixing of slot 1 air with slot 2 products
- Line c: traverses the outer premixed flame from products to reactants
- Line d: mixing of slot 2 reactants and coflowing air

Temperature vs. mixture fraction

- Evolution in reactant composition



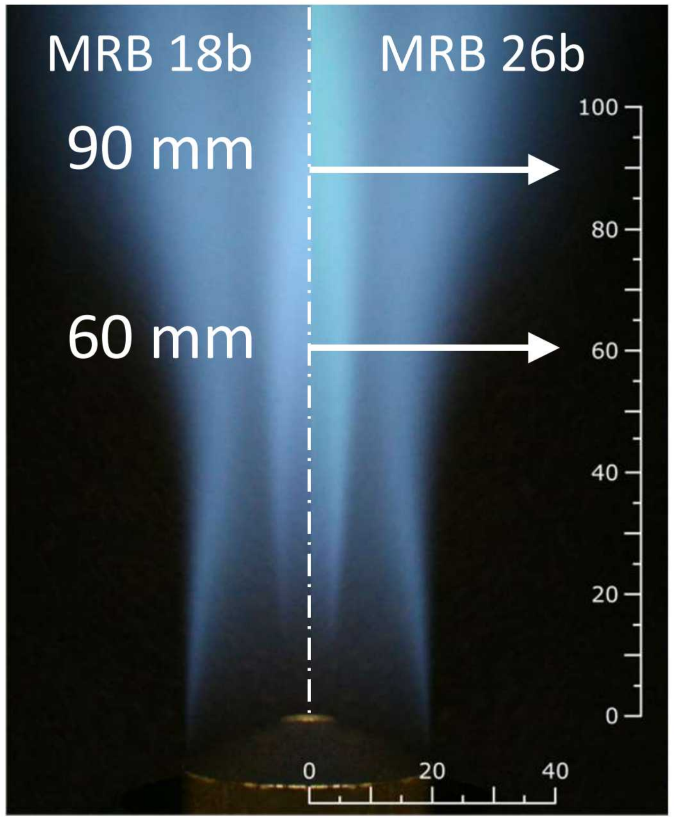
flammability limits

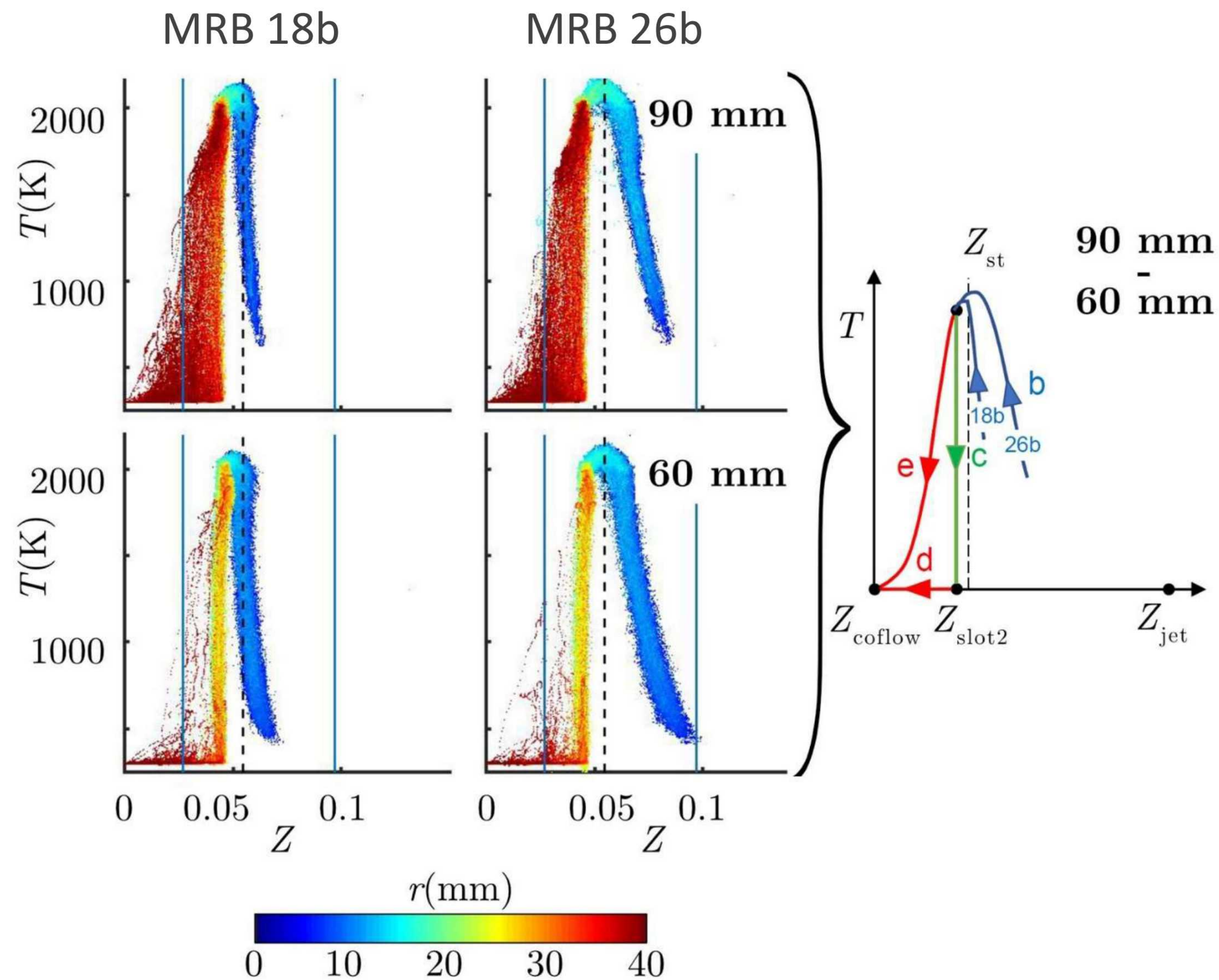


- Many samples reacting within flammability limits; lean and rich trajectories (illustrated by b_l … b_r)

Temperature vs. mixture fraction

- Smaller Z gradient in MRB18b



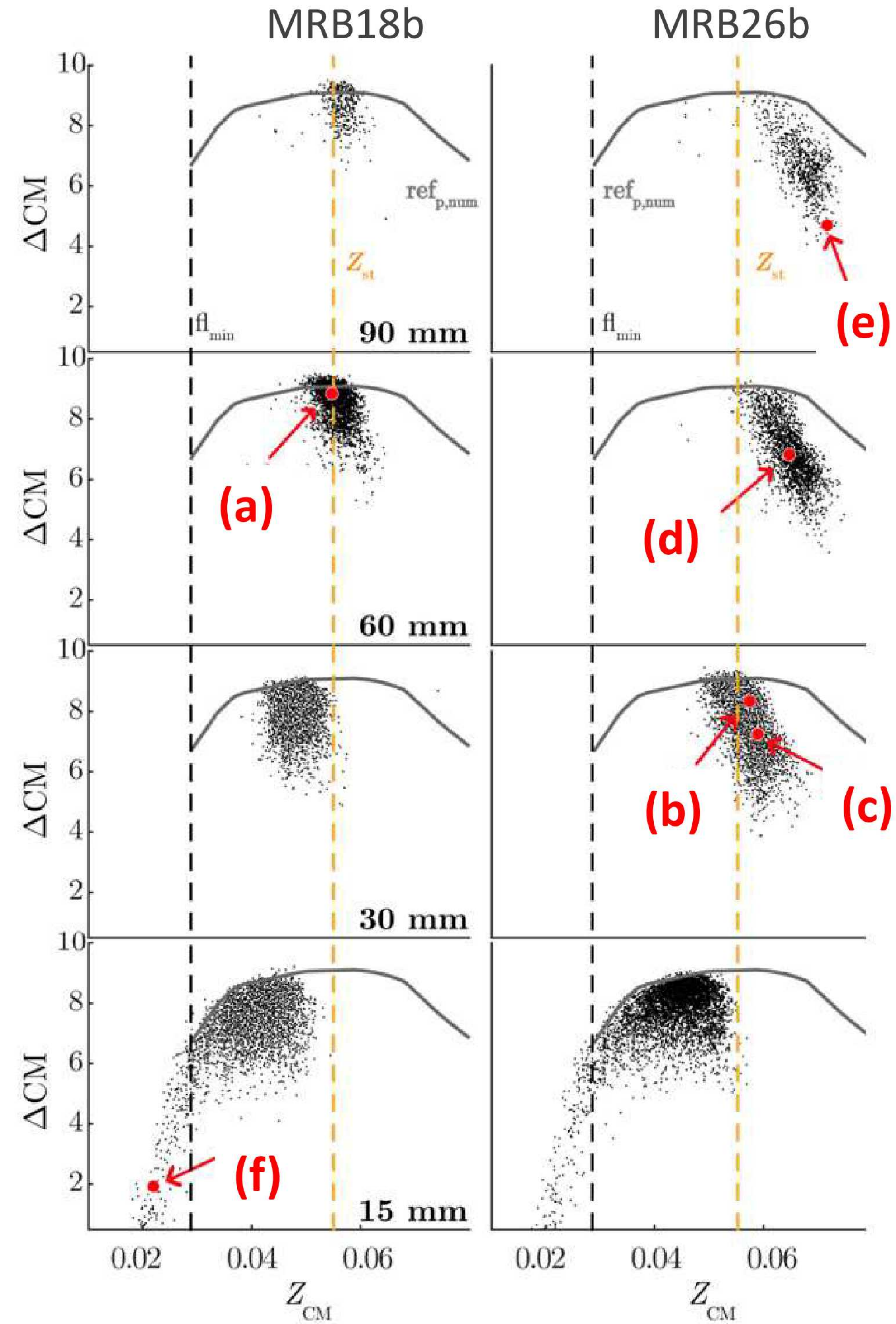


- Line e: mixing of slot 2 products and coflow air

Behavior of ΔCM

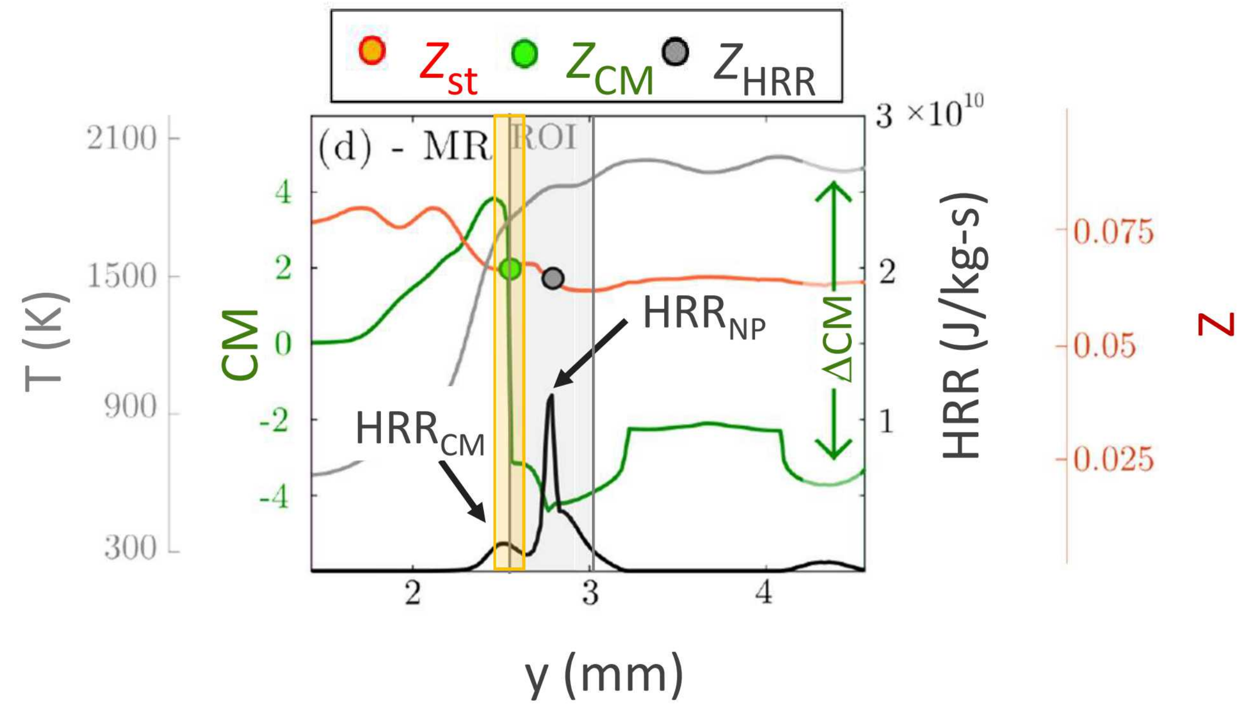
- Line shows ΔCM from premixed reactant-to-product flame calculations
- Each (ΔCM, Z_{CM}) point represents a CM zero crossing (premixed reaction zone)
- Premixed zones in the turbulent flames tend to be weaker than in laminar calculations

- Six labeled samples with decreasing ΔCM
  - (a) **premixed** reaction zone, stoichiometric
  - (b) **dominantly premixed**, slightly rich
  - (c) **multi-regime**, premixed *and* non-premixed zones
  - (d) **multi-regime**, premixed *and* non-premixed zones
  - (e) **dominantly non-premixed**, very weak premixed
  - (f) **lean back-supported** zone outside lean limit



Criteria for characterizing reaction zones

- Sample (d) multi-regime
- Region of interest (ROI) 0.5 mm wide
- HRR_{CM} = max within ±100 μm of crossing
- HRR_{NP} = max within ROI (outside 100 μm)
- $HRR_{max} = \max(HRR_{CM}, HRR_{NP})$



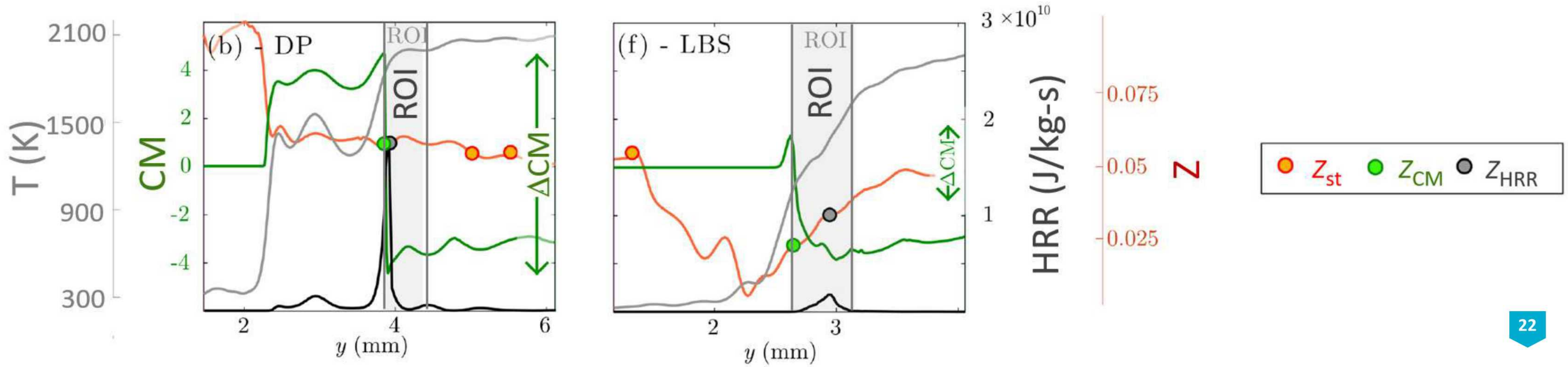
- Reaction zone index based on relative heat release:

$$\eta = (HRR_{CM} - HRR_{NP}) / HRR_{max}$$ (1 – purely premixed, -1 – purely non-premixed)

- Multi-regime: $0.8 > \eta > -0.8$

Criteria for characterizing reaction zones

premixed	P	$\eta > 0.99$, no detectable NP character
dominantly premixed	DP	$0.99 > \eta > 0.80$
multi-regime	MR	$0.80 > \eta > -0.80$
dominantly non-premixed	DNP	$-0.80 > \eta > -0.99$
non-premixed	NP	$\eta \leq -0.99$; HRR_{max} within $0.055<Z<0.07$, no CM zero crossing
lean back-supported	LBS	$Z_{CM} < Z_{HRR} < Z_{slot\ 2}$ (special case)



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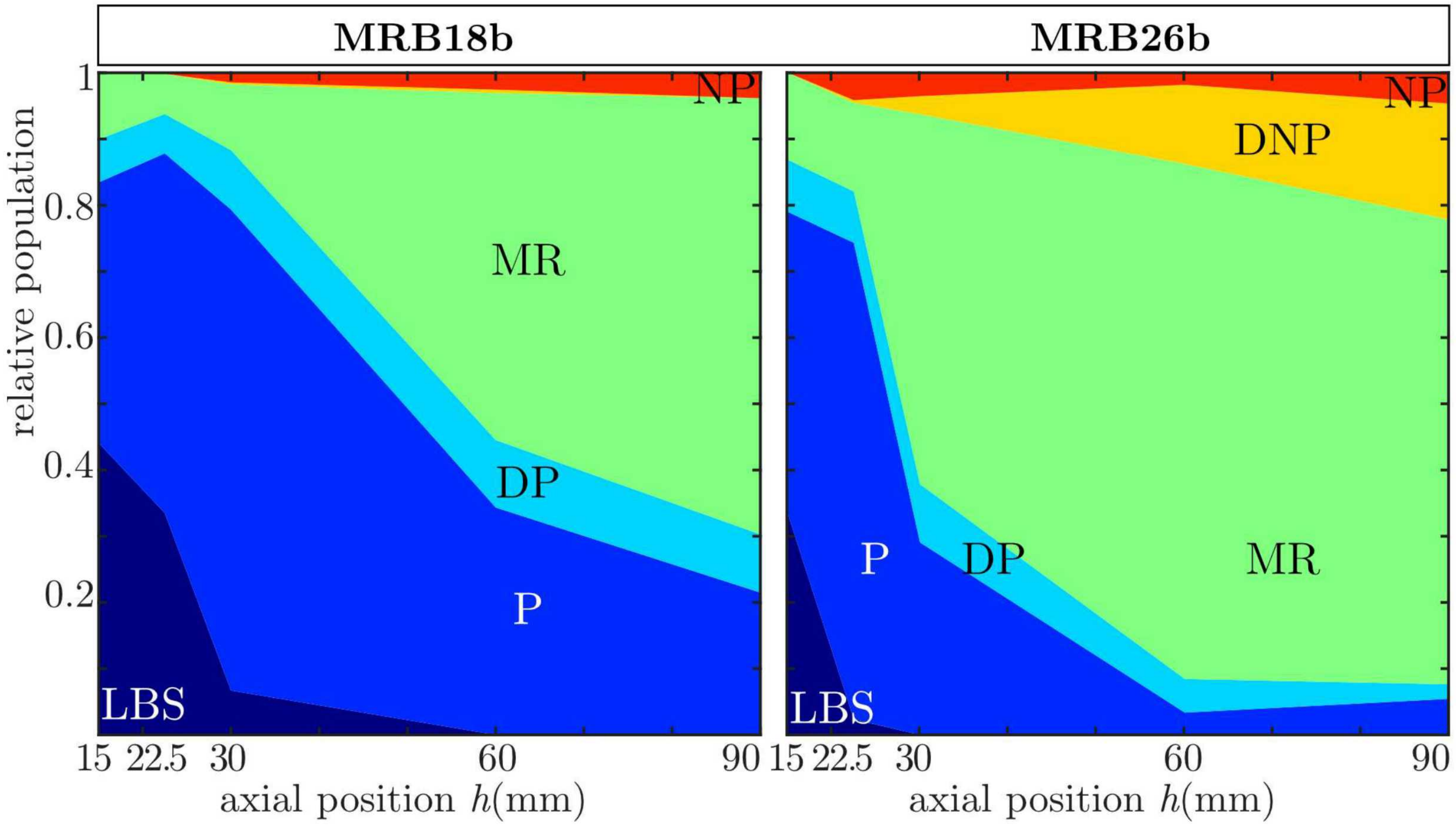
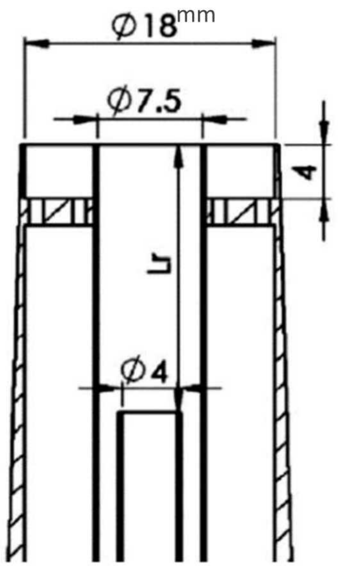
Population distribution of reaction zone structures

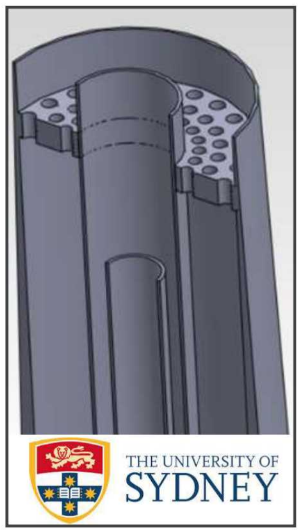


- Near field primarily premixed and stratified premixed structures in both flames (P, DP, LBS)
- Increasing probability of multi-regime (MR) structures with downstream distance, especially in MRB26b (up to 75%)
- Fully non-premixed structures are rare in both flames
- Results are not highly sensitivity to characterization parameters

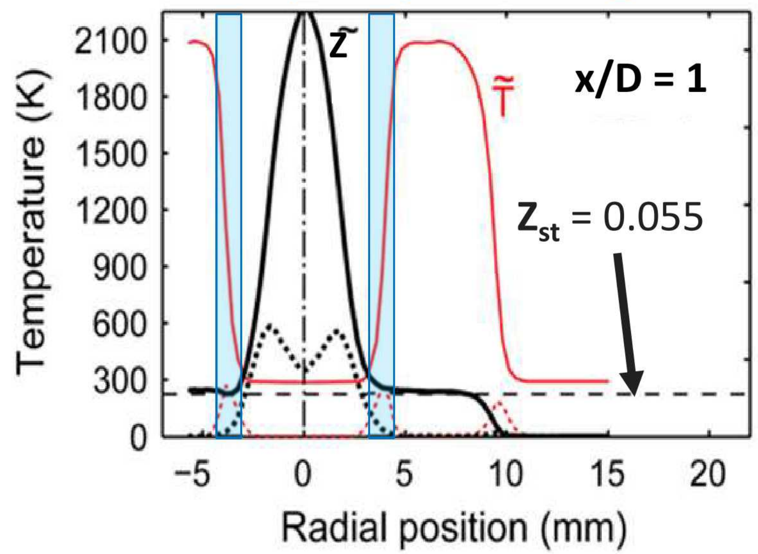
Novel capability for understanding reaction zone structures in complex turbulent flames

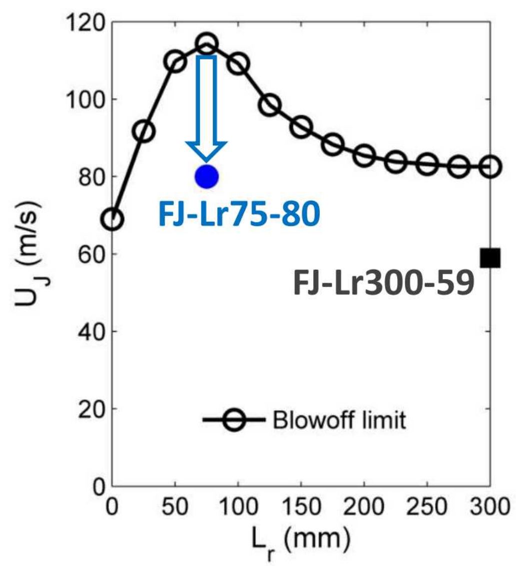
Sydney piloted inhomogeneous jet flame

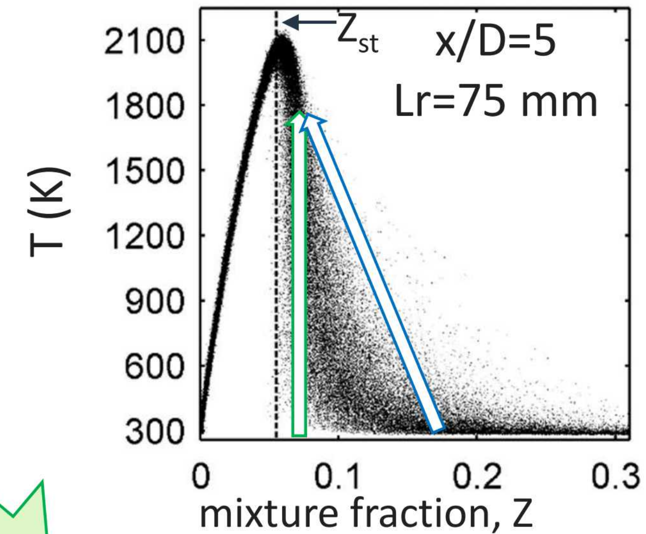


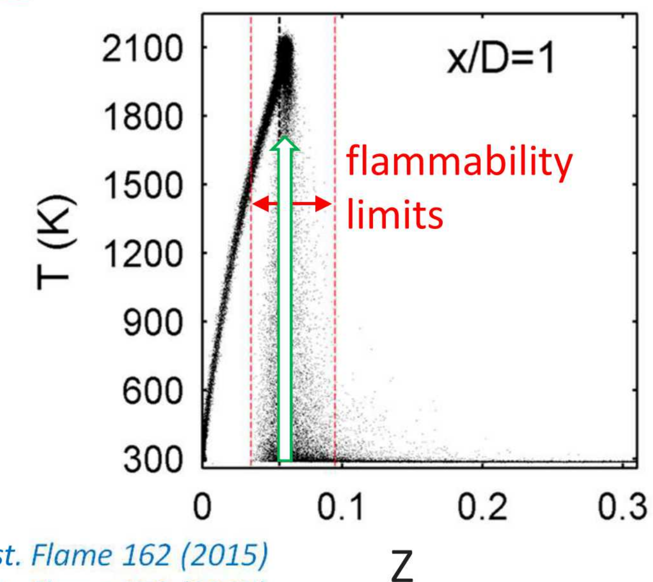


Lr=75 mm, 80 m/s "inhomogeneous"









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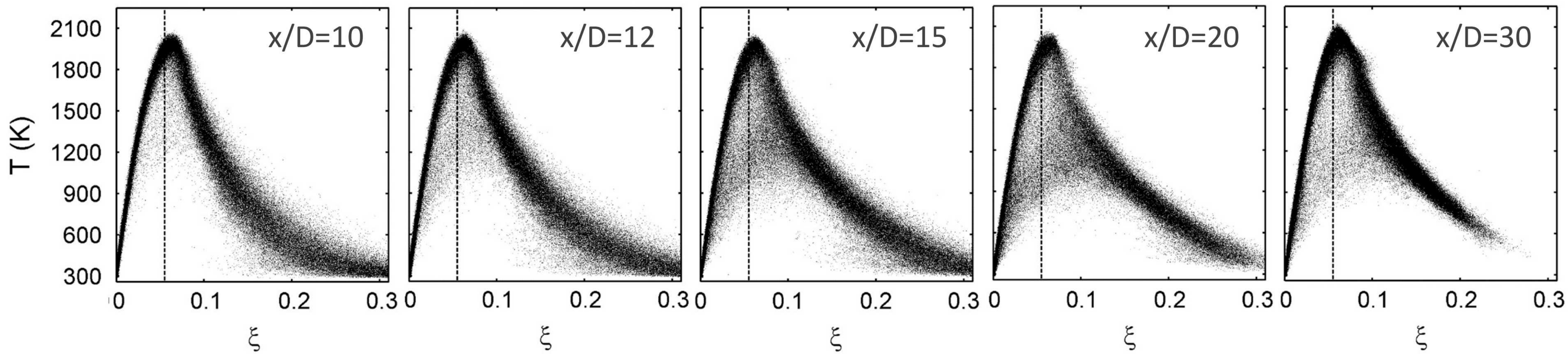
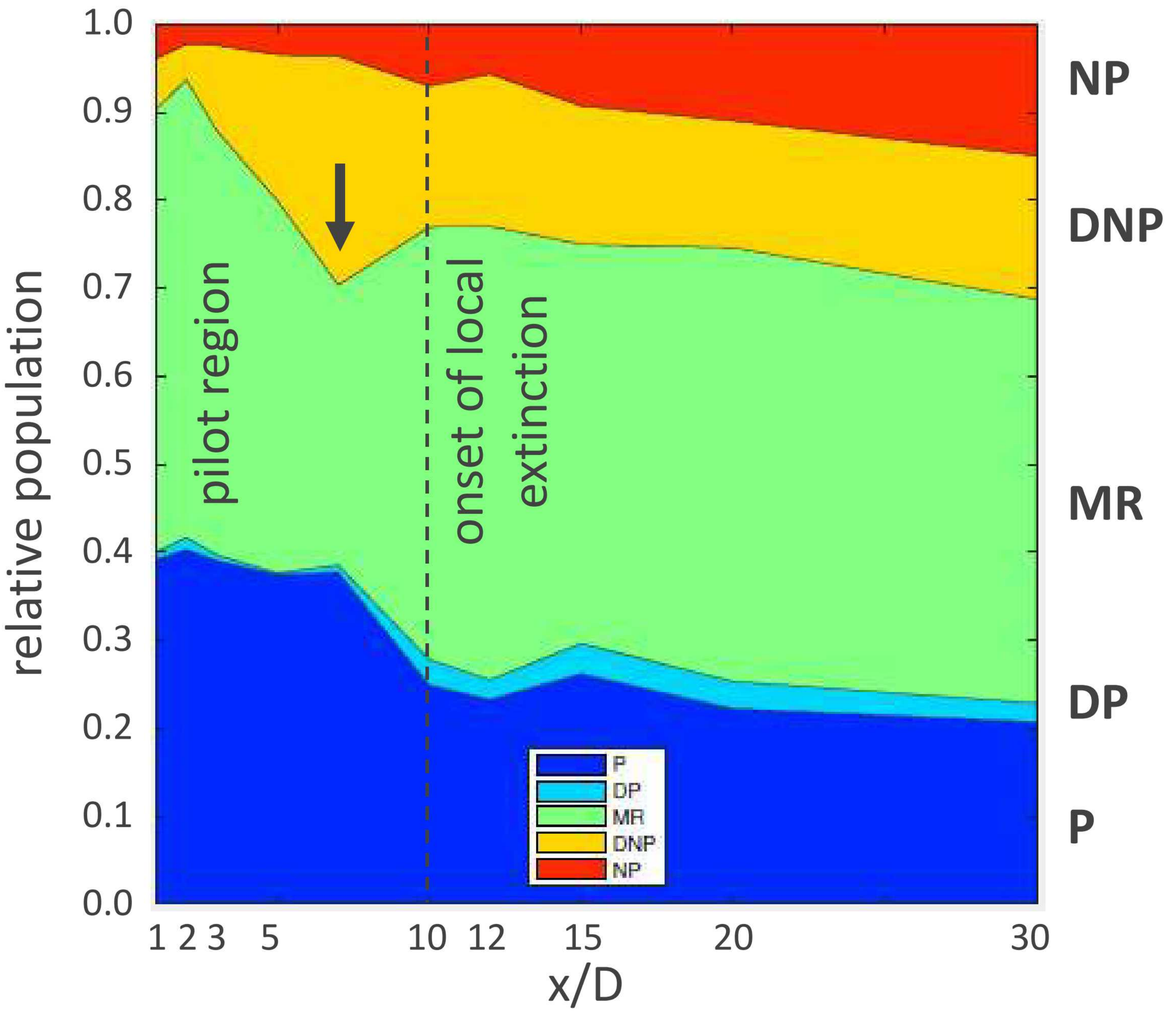
Meares et al., Proc. Combust. Inst. 35 (2015); Barlow et al. Combust. Flame 162 (2015)
Cutcher et al., Proc. Combust. Inst. 36 (2017); Barlow et al. Combust. Flame 179 (2017)

Local extinction in Sydney flame FJ-Lr75-80



- Scatter plots of temperature vs. mixture fraction
- Significant local extinction starting from x/D = 10; greatest for x/D = 15, 20
- Many partially reacted samples mixing with products within flammability limits
- **GFRI analysis can provide new insights on multi-regime combustion in flames with local extinction**

Population distribution of reaction zone structures: FJ-Lr75-80



- Mainly premixed and multi-regime flame structures in pilot region
- Increase in dominantly non-premixed reaction zones at x/D = 7; after pilot, before onset of local extinction
- Gradual increase in non-premixed structures and decrease in premixed structures with downstream distance
- Fraction of multi-regime structures is nearly 0.5 throughout the region of local extinction/re-ignition
- **New fundamental insights on reaction zone characteristics in turbulent partially premixed flames with local extinction**

Summary

- Partially premixed flames can have complex structures that combine characteristics of both premixed and non-premixed reaction zones in close proximity
- GFRI approach of approximating the full thermochemical state (and CM, HRR) starting from measured T and major species, has been extended to allow automated characterization of reaction zones
  - Criteria based on spatial proximity and relative heat release rates
  - $\eta = (HRR_{CM} - HRR_{NP}) / HRR_{max}$ (1 – purely premixed, -1 – purely non-premixed)
  - Multi-regime: $0.8 > \eta > -0.8$
- Method applied to TU Darmstadt multi-regime burner (MRB) and Sydney piloted inhomogeneous jet flame
  - MBR26b flame had up to 75% of sampled flame structures characterized as multi-regime
  - Sydney FJ-Lr75-80 flame showed ~50% multi-regime throughout region of local extinction;
    - structure is more complex than initial interpretation as evolution from premixed to non-premixed
    - (*results from last week, more work and interpretations to come*)
- Novel capability for characterizing complex reaction zones based on experimental data

Outlook

- Analysis using DNS data shows potential for significant improvement in accuracy of HRR if quantitative OH is included with T and major species as input to the homogeneous reactor calculation (Hartl et al., recently submitted)
- System for line-imaged OH LIF implemented; data sets taken during July 2018 with Dirk Geyer and Matt Dunn (analysis "in progress")
- Potential to apply GFRI analysis to older data sets (e.g., Cambridge and TUD stratified flames, other Sydney cases)

Challenges

- DOE stopped funding experimental research on turbulent flames at Sandia; Turbulent Combustion Lab idle since August 2018
- Can a comparable experimental capability be built up?

Del Valle Reservoir, Livermore, California Sep 30, 2018