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1209 ~ 2009

Insights on MILD Combustion from DNS and its Modelling

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HECTOR, ARCHER – HPC support

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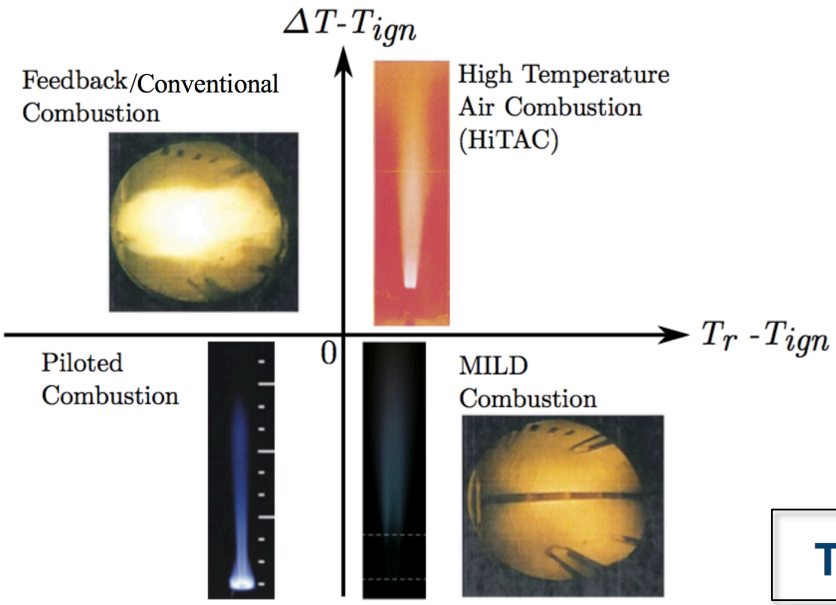
Outline

- Brief Introduction – motivation
- Methodology – DNS
- Insights gained, Examples for modelling
- Summary & Conclusion

Introduction

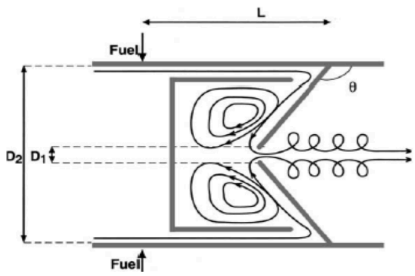
- MILD (Moderate or Intense Low-Oxygen Dilution) combustion



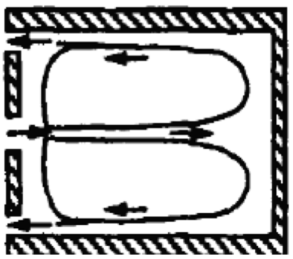
Typically Da < 1

Introduction

- Recirculation of hot gases – external or internal (internal is easy to setup without additional plumbing)



(Cavalierea, de Joannon, 2004)



(Wiinning, Wiinning, 1987)

- Staged combustion – combustion in vitiated air

- Presence of intermediate radicals in the oxidiser stream, typically O2 level < 5% by vol.

Introduction

- Advantages (“Green” combustion)

  1. Heat recovery – over all system efficiency ↑
  2. Dilution – O2 level & temperature rise drop => very low NO*x*
  3. “Silent” combustion

- Common in furnace application, considerable interest is evolving for GT by OEMs

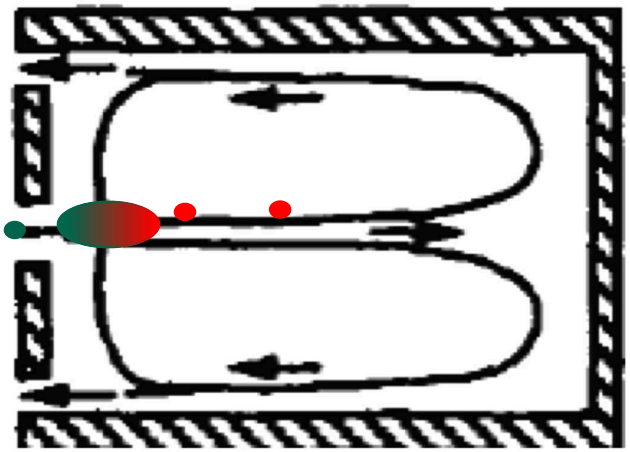
- Science – is not fully explored, perhaps not well understood yet

Objectives

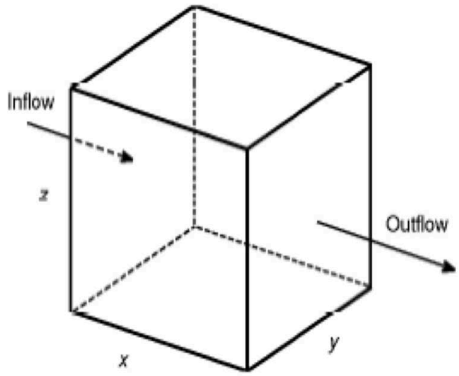
- Typical questions are

  1. Inception of MILD combustion
  2. Flame or ignition, which one is preponderant?
  3. Is it *Mixed Mode* combustion?
  4. What are typical morphological and topological features of reactions zones?
  5. Are standard experimental diagnostics (developed & tested using typical flames) adequate?
  6. … etc., & of course, what is correct modelling approach?

DNS Amenable Configuration – Schematic

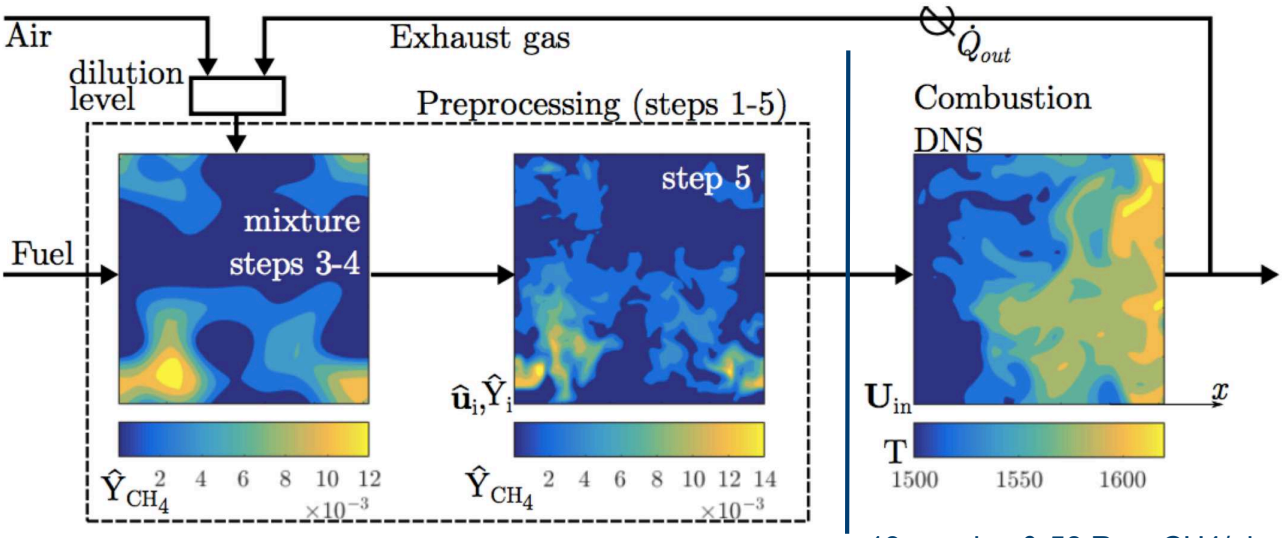


Computational Domain for **DNS**



Methodology – Inflowing Mixture

(PROCI 2012, CnF 2014, CnF 2018)

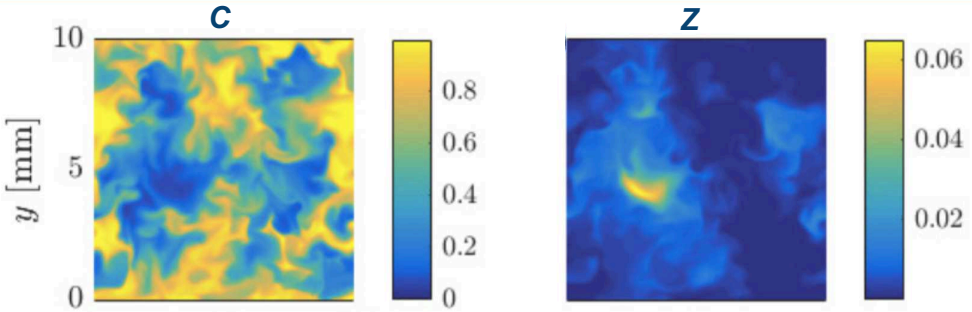


Step 1: Turbulence field generation
Step 2 to 4: Scalar fields generation
Step 5: tying turbulence & scalar fields together for consistencies

19 species & 58 Rxn CH4/air chemistry
Includes OH* chemistry
512x512x512
First of its kind simulation

Inflowing Mixture

(CnF 2018, 189, 173-189)

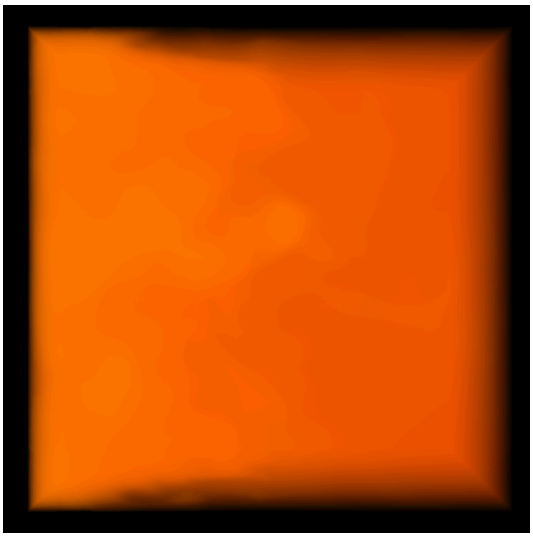


$0 \leq \phi \leq 11$

$Y_i\,(Z, c)$

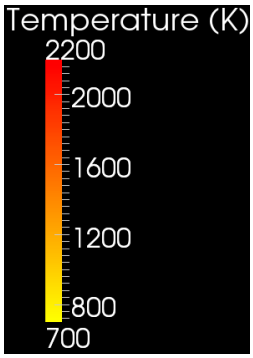
MILD vs Conventional Comb. – from DNS

(CST 186, p. 1075 2014)



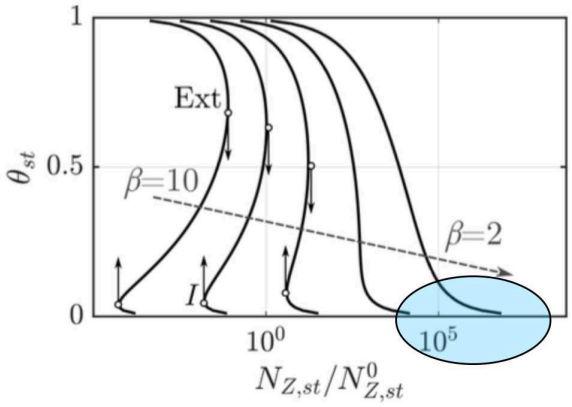
MILD

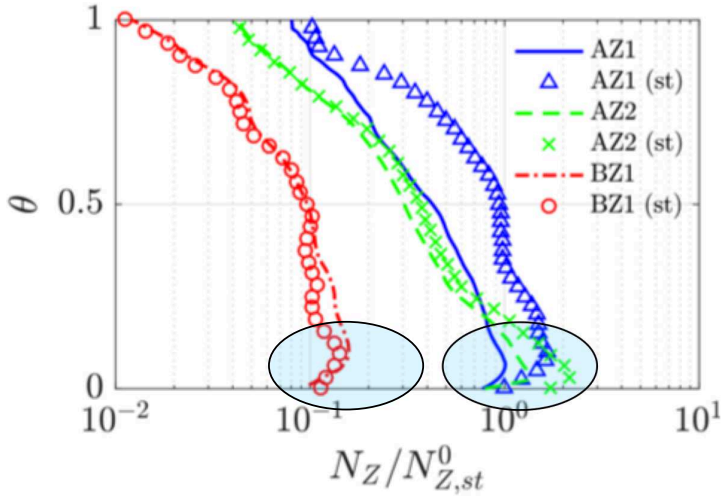
Conventional – lean premixed



MILD Combustion Inception

(Doan & Swaminathan PROCI 2019)



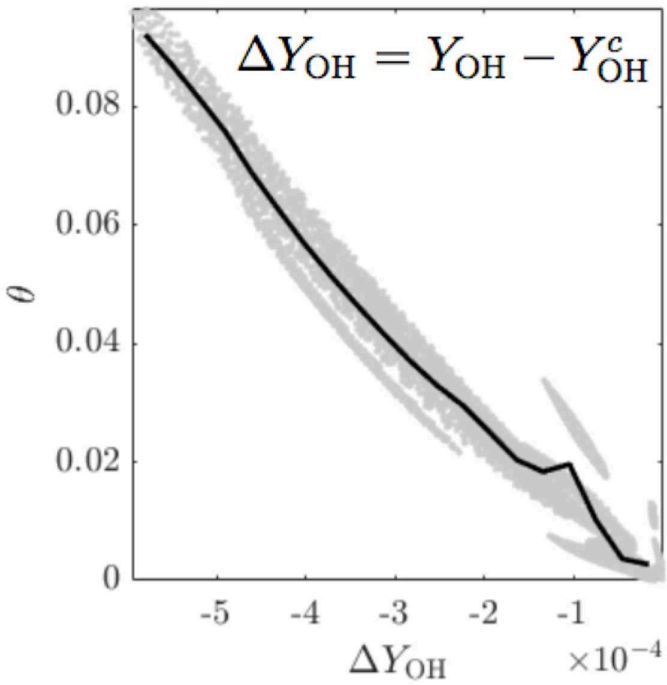


$$\theta_{st} = (T_{st} - T_{st,u})/\Delta T_{st}$$

$$\beta = E_{eff}/(R^0 T_{st,b}) = T_a/T_{st,b}$$

MILD Combustion Inception

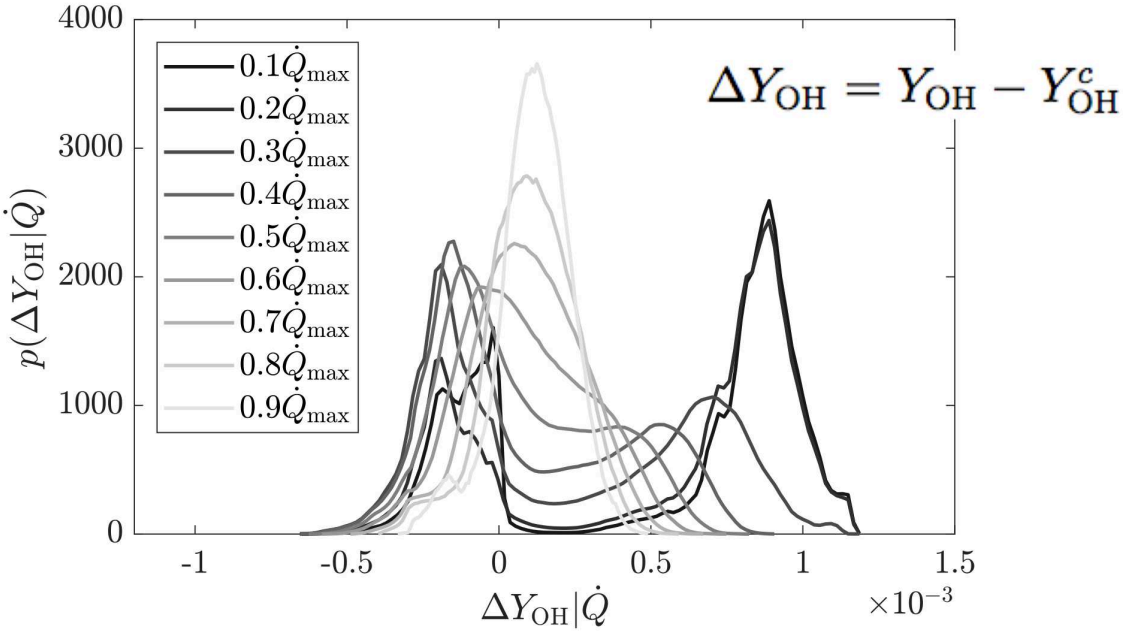
(Doan & Swaminathan PROCI 2019)



- Radicals in the incoming flow play important role in initiating the combustion
- Revised theory for S-type curves under MILD conditions – open question

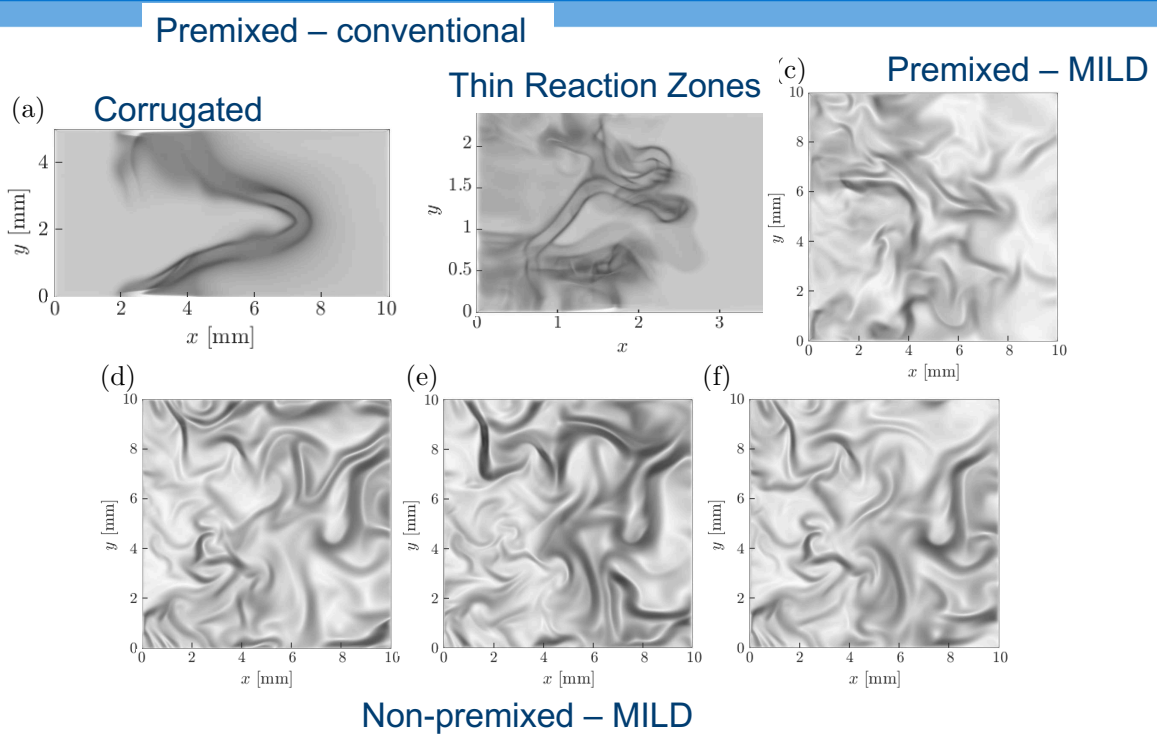
Note on the OH LIF for MILD Cond. – 1

(CST 2019 in Reviesed)

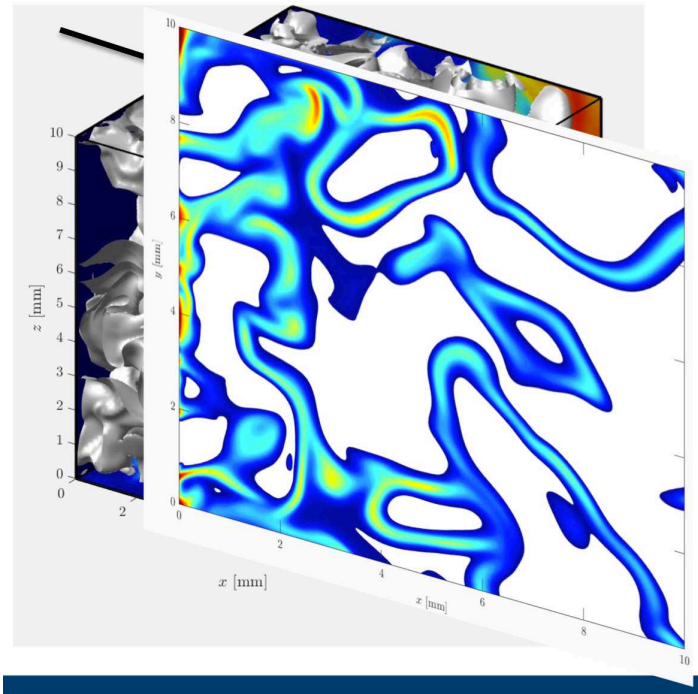


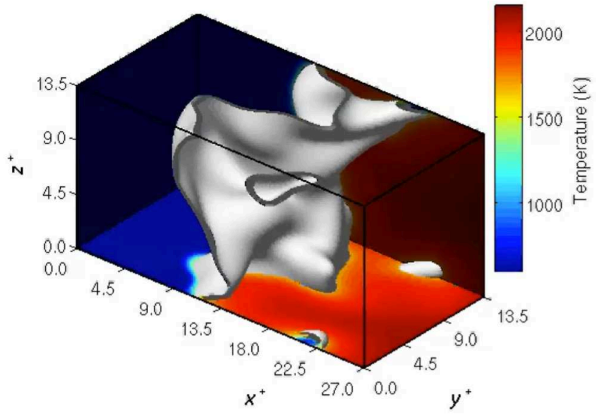
Note on the OH LIF for MILD Cond. – 2

(CST 2019 in Revised)



Visualisation

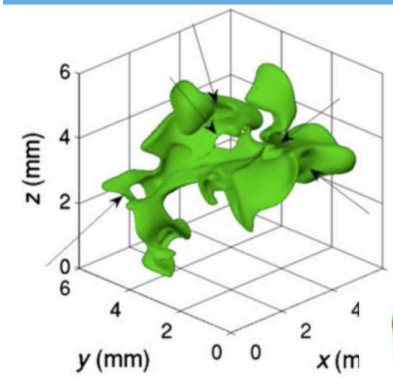


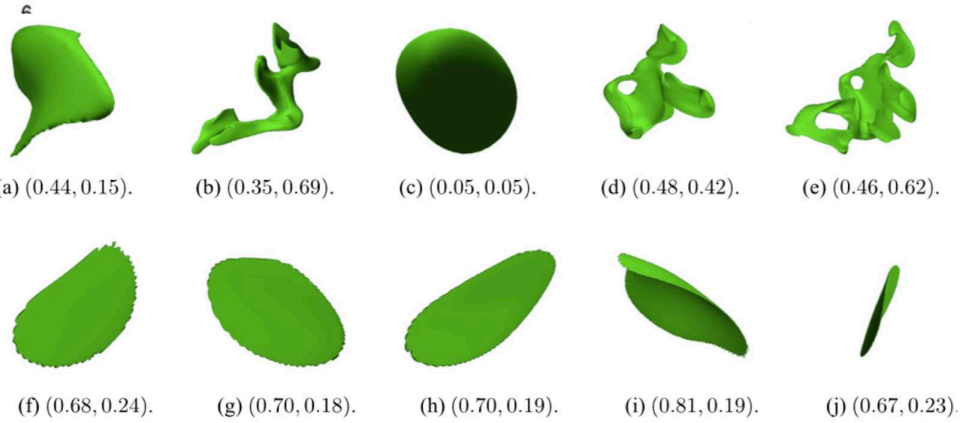


- Complex topology & morphology
- Interacting reaction zones
- Complex dynamics
- How to describe these structures?

Morphology of Rxn Zones

(CnF 2014, 161, 2801-2814)





(a) (0.44, 0.15). (b) (0.35, 0.69). (c) (0.05, 0.05). (d) (0.48, 0.42). (e) (0.46, 0.62).

(f) (0.68, 0.24). (g) (0.70, 0.18). (h) (0.70, 0.19). (i) (0.81, 0.19). (j) (0.67, 0.23).

Morphology Characterisation

(Leung et al. JFM 710, 2012, 453-481)

N dimensional object has (N+1) Minkowski Functionals : from Integral Geomery

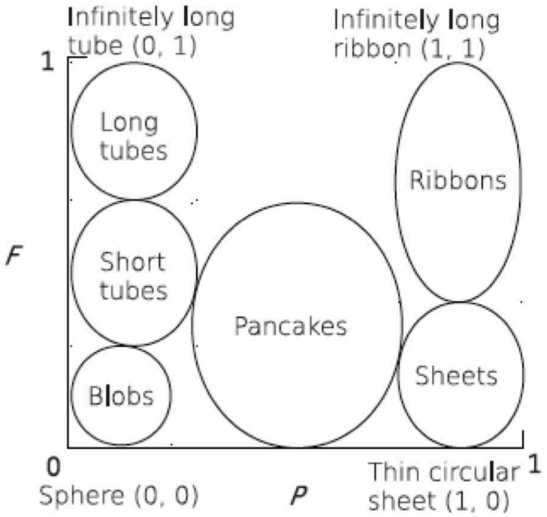
$$\mathcal{F}_0 = \mathcal{V}, \quad \mathcal{F}_1 = \frac{\mathcal{S}}{6}, \quad \mathcal{F}_2 = \frac{1}{3\pi}\int_S \frac{\kappa_1+\kappa_2}{2}\, dS, \quad \mathcal{F}_3 = \frac{1}{2\pi}\int_S \kappa_1\kappa_2\, dS,$$

$$\text{Thickness, } T \equiv \frac{\mathcal{F}_0}{2\mathcal{F}_1}; \quad \text{Width, } W \equiv \frac{2\mathcal{F}_1}{\pi\mathcal{F}_2}$$

$$\text{Length, } L \equiv \frac{3\mathcal{F}_3}{4(G+1)} \quad G = 1 - 0.5\mathcal{F}_3$$

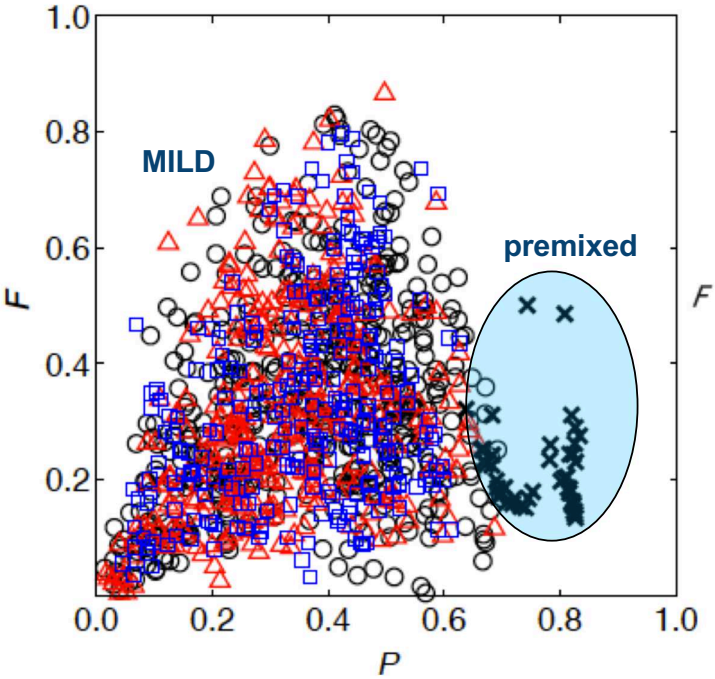
$$\text{Planarity, } P \equiv \frac{W-T}{W+T}$$

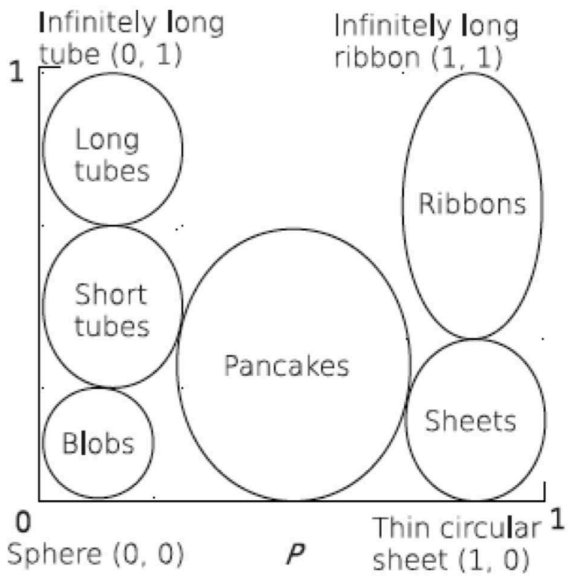
$$\text{Filamentarity, } F \equiv \frac{L-W}{L+W}$$



Morphology of Reaction Zones

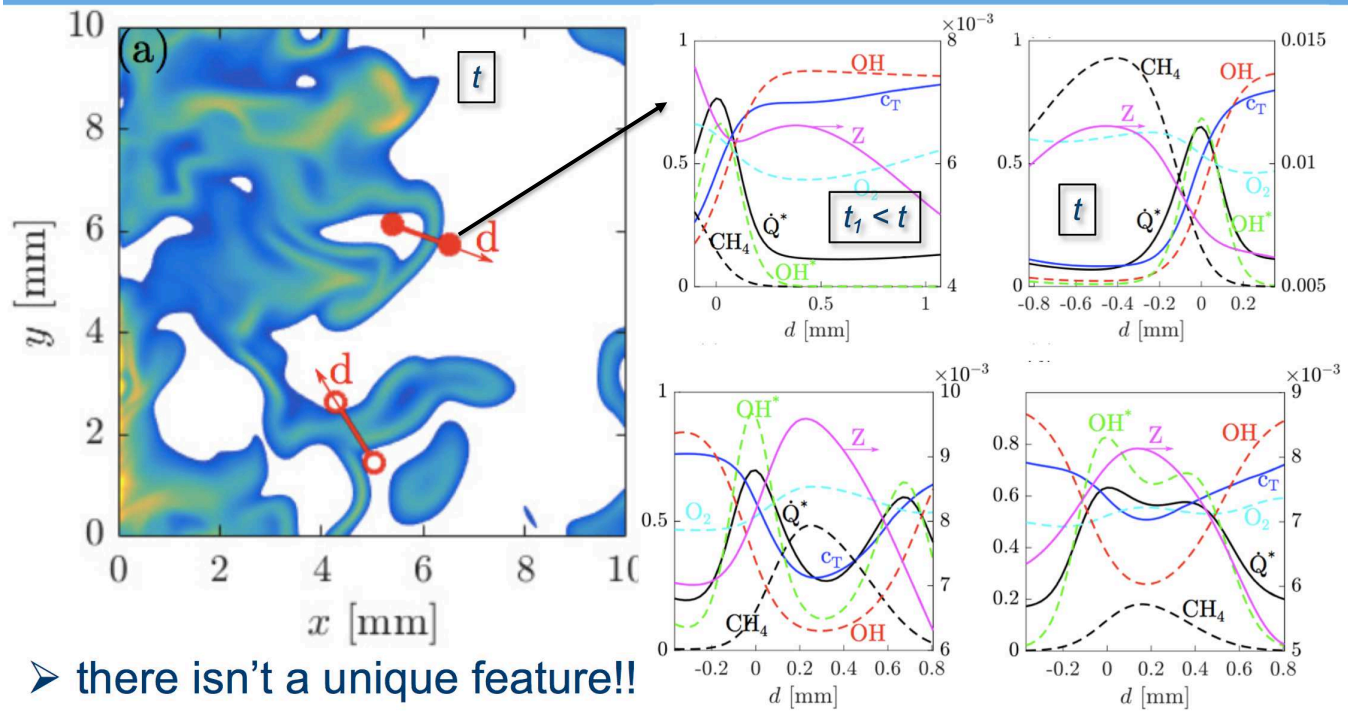
(CnF 2014, 161, 2801-2814)





How do We Characterise the Structure?

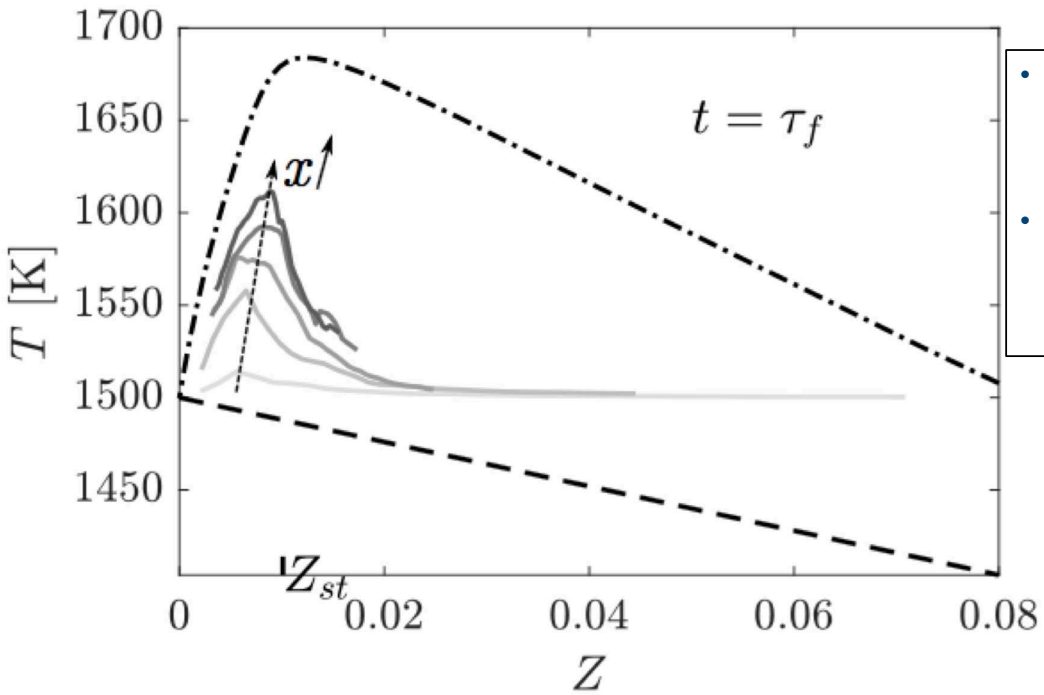
(CnF 2018, 189, 173-189)



➢ there isn't a unique feature!!

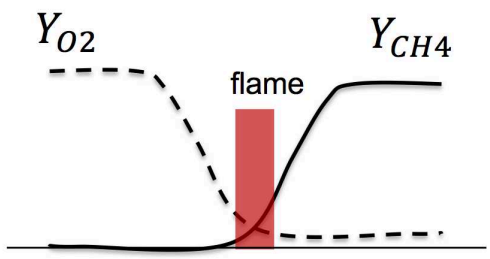
Mixture Fraction Space Structure

(CnF 2018, 189, 173-189)

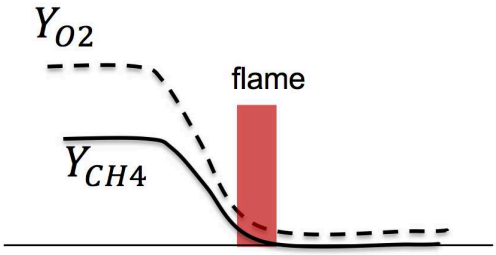


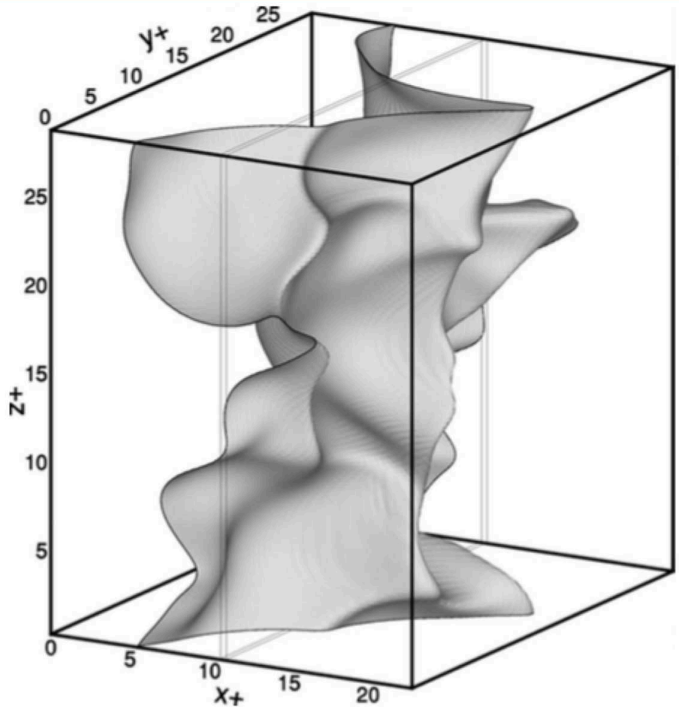
- Spatial /temporal propagation of Autoignition front
- Some features of flames – both premixed and non-premixed

How About Scalar Gradient?



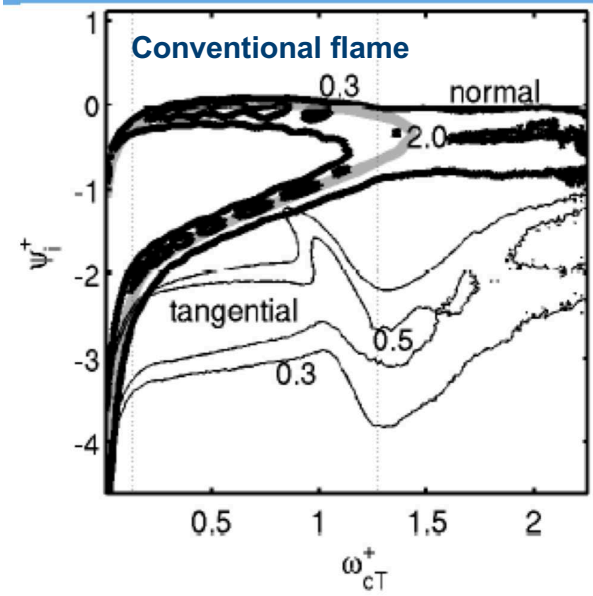
Flames:
normal gradient >> tangential gradients

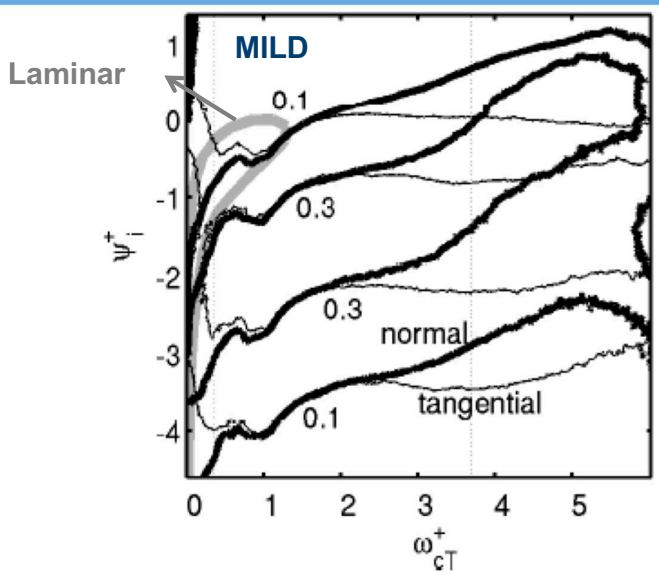




Scalar Gradients & Rxn. Rate – JPDF

(CnF 2014, 161, 1063-1075)





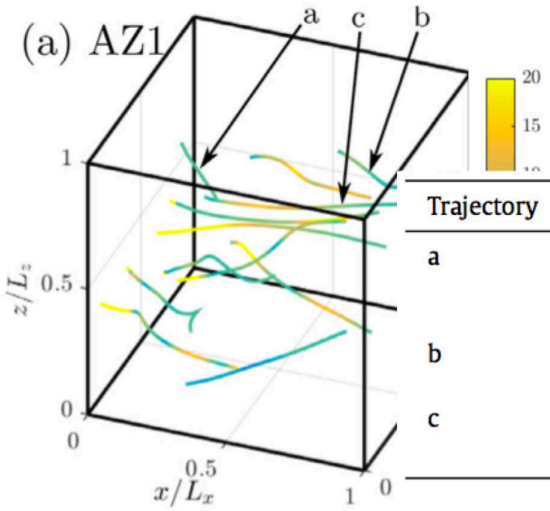
Shares some common features with conventional combustion, while having some distinctive features

Flame or Ignition? – $\mathcal{B}$ Analysis

(CnF 2014, 161, 2801-2814) (CnF 2019, 201, 234-243)

$$\frac{\partial \rho Y_\alpha}{\partial t} + \underbrace{\frac{\partial \rho u_j Y_\alpha}{\partial x_j}}_{\mathcal{C}\text{: conv.}} = \underbrace{\frac{\partial}{\partial x_j}\left(\rho D_\alpha \frac{\partial Y_\alpha}{\partial x_j}\right)}_{\mathcal{D}\text{: diff.}} + \underbrace{\dot{\omega}_\alpha}_{\mathcal{R}\text{: react.}}$$

$$\mathcal{B} = |\mathcal{C} - \mathcal{D}| - |\mathcal{R}|$$



Variety of scenario is observed

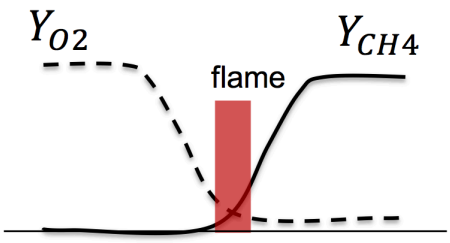
Trajectory	AZ1, Fig. 5	AZ2, Fig. 6	BZ1, Fig. 7
a	Ignition of lean mixture evolving into flame	Sequential ignition of stratified lean mixtures	Lean ignition
b	Ignition of rich mixture	Ignition of rich mixture	Lean ignition evolving into flame
c	Unsteady rich flame		

Flame Index Analysis

$$\mathrm{FI} = \frac{Z - Z_{st}}{2|Z - Z_{st}|}\left(1 + \frac{\nabla Y_{CH_4} \cdot \nabla Y_{O_2}}{|\nabla Y_{CH_4}||\nabla Y_{O_2}|}\right)$$

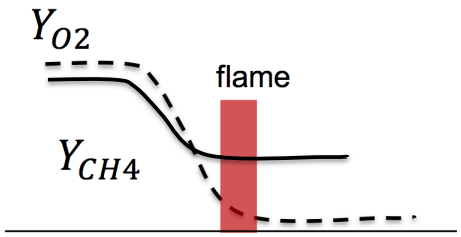
(Briones et al. Phys. Fluids 2006)

= 0 for non-premixed



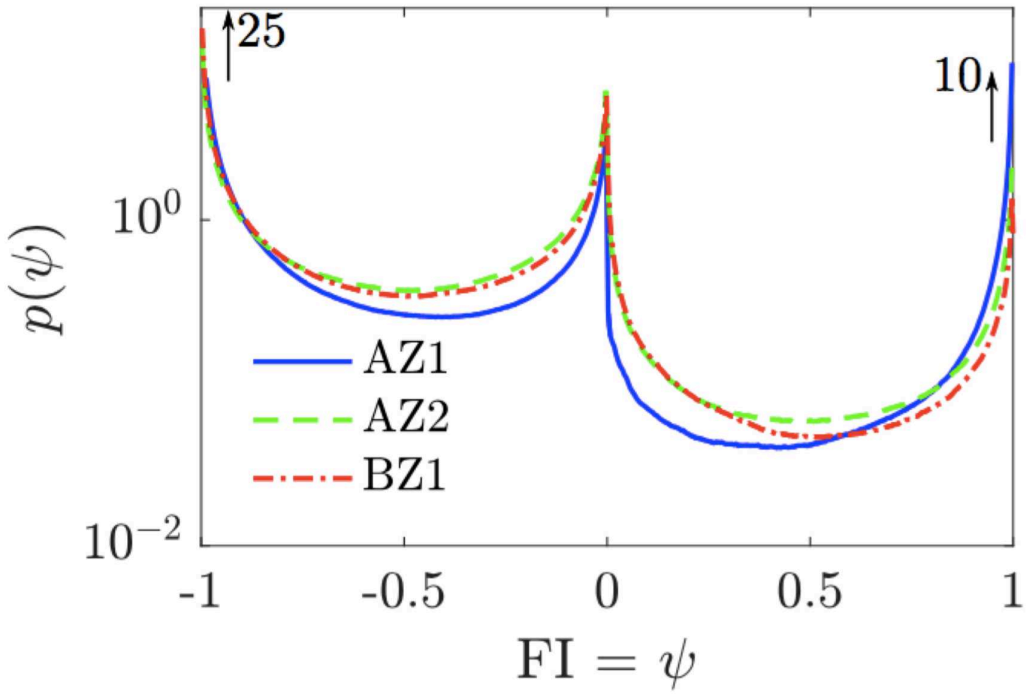
= 1 for rich premixed

= -1 for lean premixed



PDF of FI

(CnF 2018, 189, 173-189)



Relative contributions of LP, RP, NP, & MM

(CnF 2018, 189, 173-189)

$$\mathcal{V}_{NP} = \int_{-\xi_1}^{\xi_1} p(\psi)\, d\psi \quad \mathcal{V}_{LP} = \int_{-1}^{-\xi_2} p(\psi)\, d\psi \quad \mathcal{V}_{RP} = \int_{\xi_2}^{1} p(\psi)\, d\psi$$

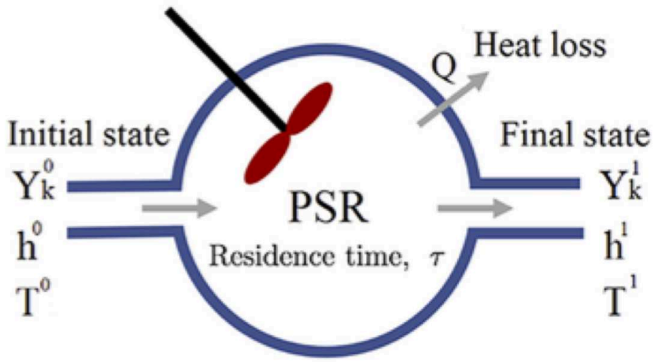
Case	$\mathcal{V}_{NP}$	$\mathcal{V}_{RP}$	$\mathcal{V}_{LP}$	$\mathcal{V}_{MM}$	$\mathcal{Q}_{NP}$	$\mathcal{Q}_{RP}$	$\mathcal{Q}_{LP}$	$\mathcal{Q}_{MM}$
AZ1	0.13	0.13	0.52	0.22	0.114	0.134	0.504	0.248
AZ2	0.28	0.07	0.37	0.28	0.230	0.027	0.499	0.244
BZ1	0.26	0.05	0.44	0.25	0.206	0.026	0.533	0.235

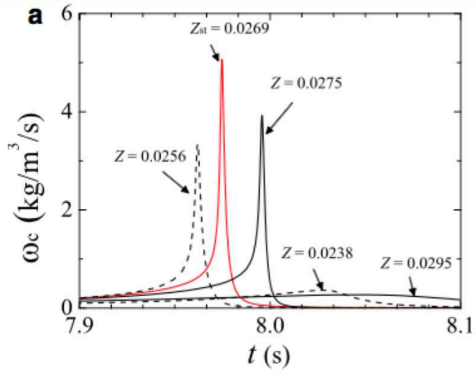
Modelling – Reaction rate

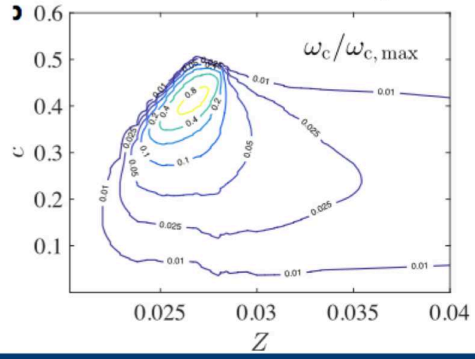
(PROCI, 36, 2017, 4279-4286)

$$\overline{\dot{\omega}_c^-} = \iiint \dot{\omega}_c^-(\xi, \eta, \zeta) P(\xi, \eta, \zeta)\, d\xi\, d\eta\, d\zeta$$

$$P(\xi, \eta, \zeta) = \beta(\xi; \tilde{Z}, \tilde{Z}''^2)\delta(\eta - \tilde{h})\beta(\zeta; \tilde{c}, \tilde{c}''^2)$$

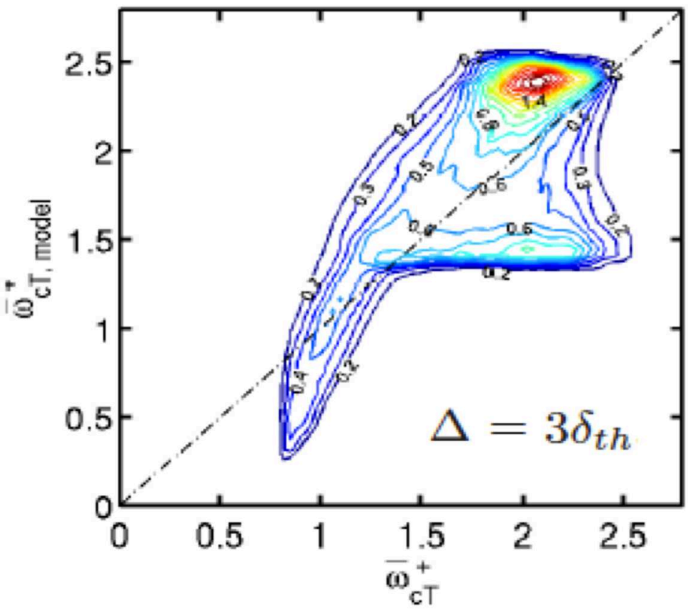






Modelling – Reaction rate

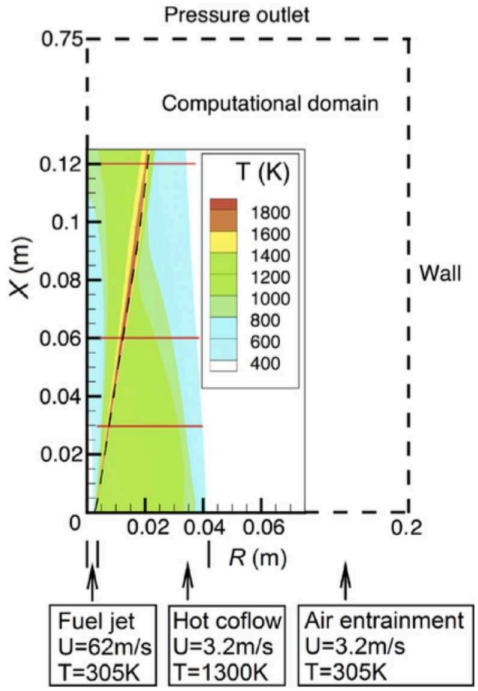
(PROCI, 35, 2015, 3529 - 3536)

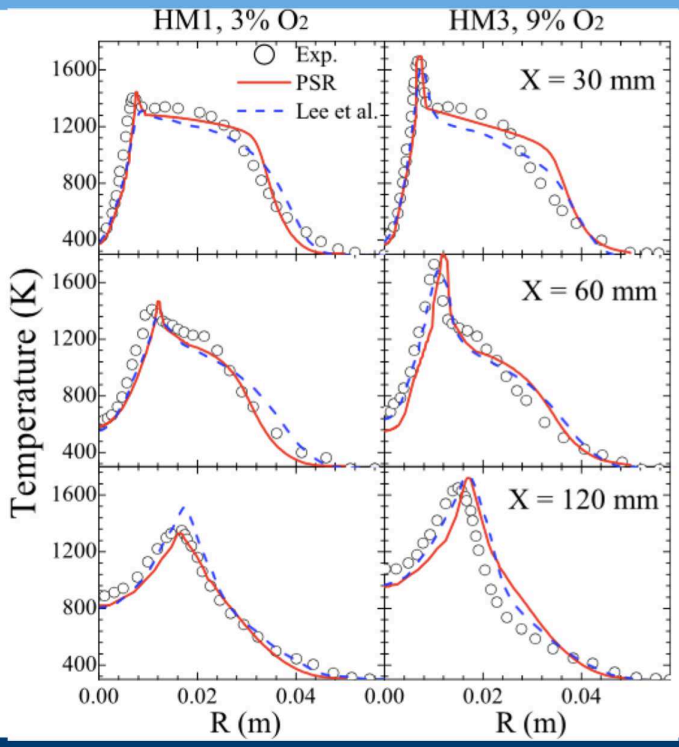


Minamoto & Swaminathan, Int. J. Adv. Eng. Sci. Appl. Math 2014, 6, p. 65

Validation – RANS – Adelaide JHC

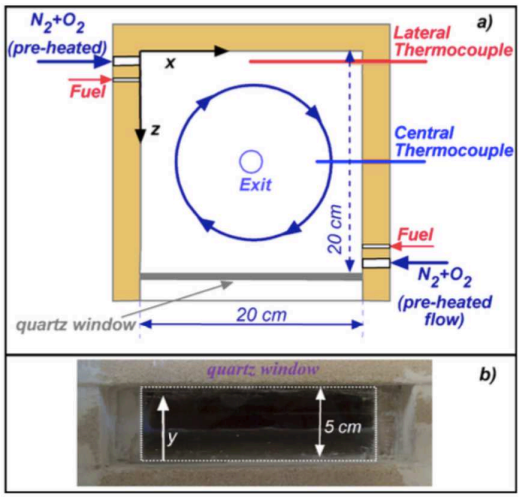
(PROCI, 36, 2017, 4279-4286)

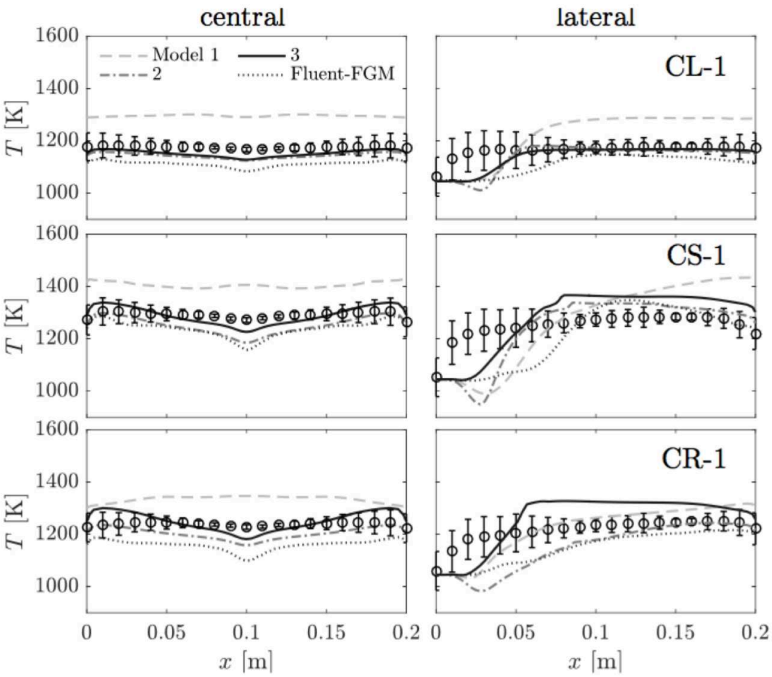




Validation – RANS – Naples Cyclone burner

(Energy & Fuel 32, 2018,10256-10265)





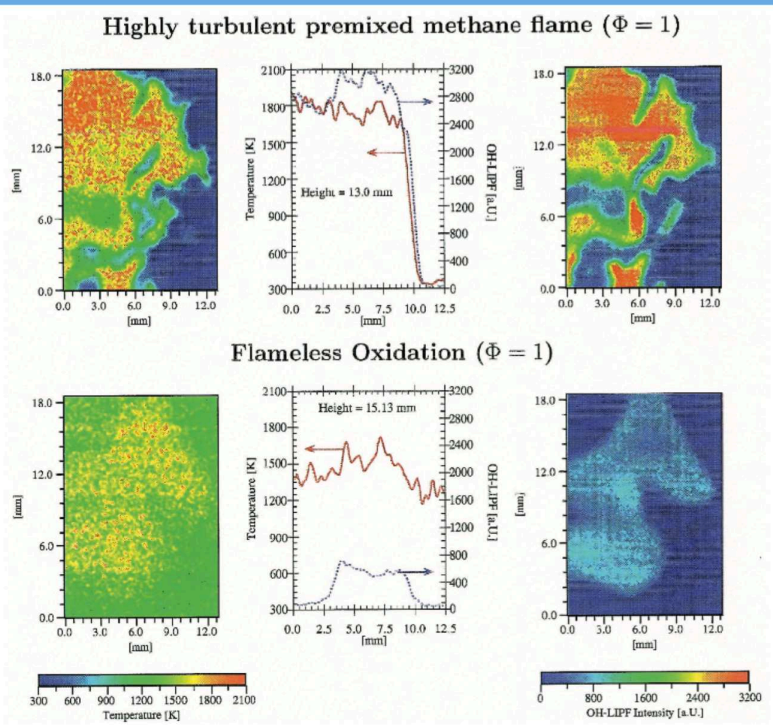
Summary & Conclusion

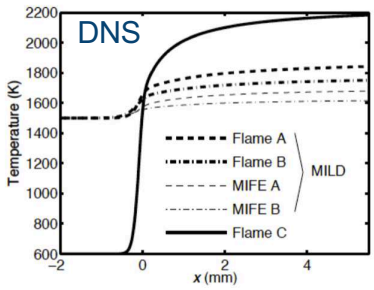
- MILD combustion involves complex interactions among auto-ignition fronts, premixed and non-premixed flames
- Thus, it shares some commonality with conventional combustion while having its distinctive attributes
- S-shaped curve – need revision for MILD condition
- Rxn zones have pancake like structures with typical thickness of about $\delta_{th}/10$

Summary & Conclusion

- Standard surface based combustion modelling is inadequate
- Reactor based modelling approach seems to be suited well
- Validated this for RANS
- Tested for LES (*a priori*), further work is on-going
- Need to be careful while interpreting LIF images of MILD conditions

Questions?


Highly turbulent premixed methane flame (Φ = 1)
Height = 13.0 mm
Temperature [K]
OH-LIPF [a.U.]
[mm]
Flameless Oxidation (Φ = 1)
Height = 15.13 mm
Temperature [K]
OH-LIPF Intensity [a.U.]


DNS
Temperature (K)
x (mm)
Flame A
Flame B
MIFE A
MIFE B
Flame C
MILD