DNS of Partially Premixed MILD Combustion: Preliminary Investigations

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Durham University

Presentation Structure

1. Introduction
2. DNS Methodology
3. Preliminary Results
   - Morphology of Reaction Zones
   - Joint PDF of c_T and Z
4. Conclusion

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Introduction

- Combustion and fossil fuels: main source of energy for the foreseeable future
- Need to improve combustion efficiency and reduce pollutants emission
- Moderate or Intense Low-oxygen Dilution (MILD) combustion: promising concept
    - $T_r > T_{ign}$, $\Delta T < T_{ign}$, low oxygen concentration
    - Achieved by exhaust gas recirculation
    - Physics of MILD combustion: challenging
        - Spatially distributed reactions
        - No visible flame front
        - Auto-ignition phenomena and flame behaviour? Models?
- Use of Direct Numerical Simulations (DNS) to obtain physical insights

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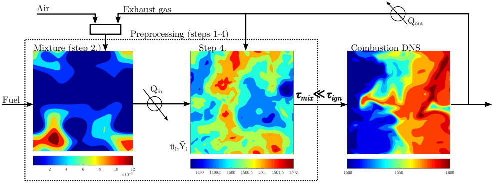
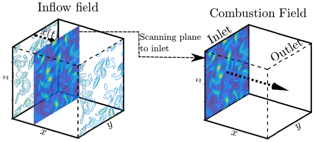
DNS Configuration

- Split of the DNS of MILD combustion into a mixing phase and a combustion phase

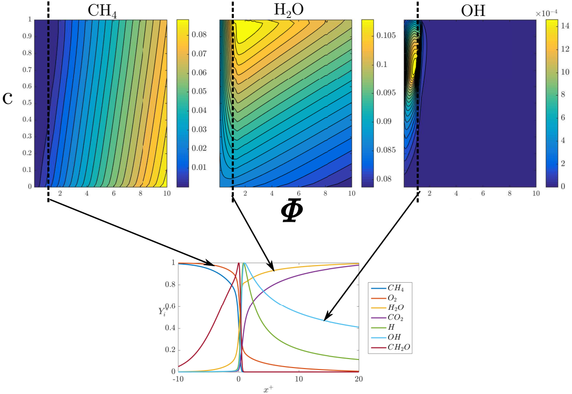


- Numerical domain: cuboid of size 10^3 mm discretized with 512^3 nodes
  - Periodic in y-z and NSCBC at the outlet
  - Inflow from preprocessed field



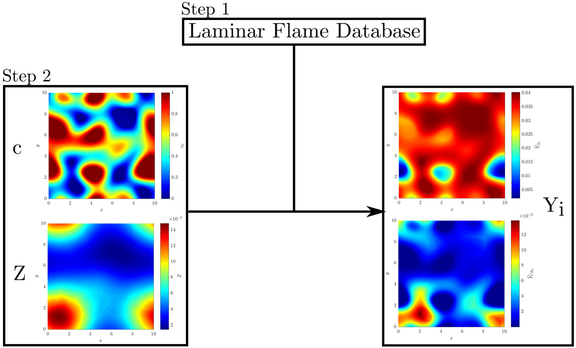
Preprocessing of Initial and Inflow Conditions

1. Database of freely propagating laminar premixed flames of methane-air diluted with products of combustion.



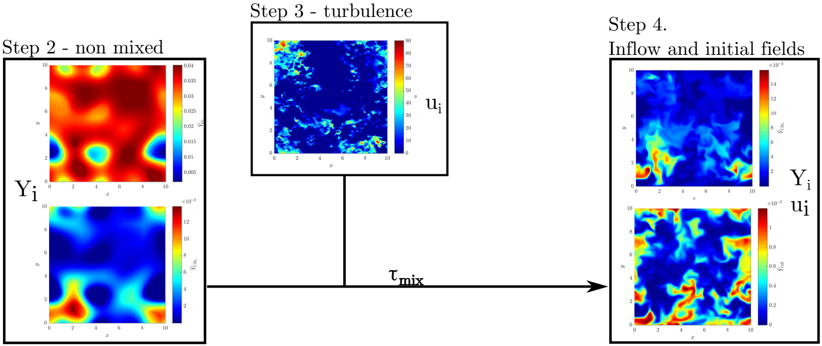
Preprocessing of Initial and Inflow Conditions

2 Construction of mixture fraction Z and progress variable c field using the methodology of Eswaran and Pope [1987]. Temperature set to an initial constant temperature T_m.



Preprocessing of Initial and Inflow Conditions

3. Generation of a freely decaying homogeneous isotropic turbulent velocity field.
4. Combination of Y_i of step 2 and turbulence field. Simulation without chemical reactions for one large eddy time.



DNS Cases

Case	$Re_{l_0(\lambda)}$	$\langle X_{O_2} \rangle$	$X_{O_2}^{\max}$	L_c/L_Z	l_0/L_Z	$\langle Z \rangle$	Z_{st}
AZ1	96 (37)	0.027	0.035	0.77	0.60	0.008	0.01
BZ1	96 (37)	0.027	0.035	1.0	0.46	0.008	0.01
AZ2	96 (37)	0.016	0.020	0.77	0.60	0.0047	0.0058

- Similar turbulence field for all cases
- Cases with $L_c/L_Z \leq 1$ chosen as chemical lengthscale smaller than mixing lengthscale but high recirculation in MILD combustion yielding $L_c/L_Z \approx 1$ possible
- Lower O_2 content $\rightarrow$ more distributed reactions [1] and recent more restrictive definition of MILD combustion [2]

[1] Minamoto & Swaminathan, CnF (2014)
[2] Evans et al. , PROCI (2016)

DNS Cases

- Chemical mechanism based on Smooke methane-air mechanism [1], extended to include OH^*-chemistry [2]: 19 species, 58 reactions
- Numerical code used: SENGA2
- Simulation parameters
  - 4096 cores (171 nodes)
  - $\Delta t = 1$ns, 750000 timesteps for 1.5 flowthrough time
  - Wall-clock time per DNS: $\sim$ 530 hours
- MAUs cost
  - 10 MAUs: Computation of turbulence field and initial tests (smaller grids...)
  - 33MAUs: Cost per DNS simulation
  - Total: $\sim$110 MAUs
- Computation time allocated
  - ARCHER RAP project: 62 MAUs
  - UKCTRF: 20 + 30 MAUs

[1] Smooke & Giovangigli, Lecture Notes in Physics (1991)
[2] Kathrotia et al., Appl. Phys. B Lasers Opt. (2012)

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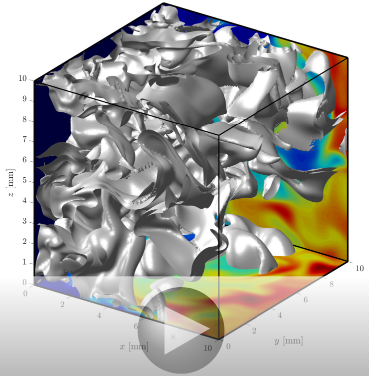
DNS of MILD Combustion

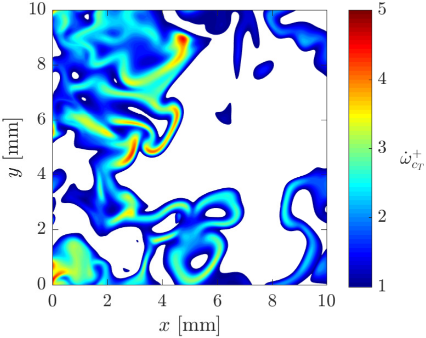


CASE AZ1

$\langle X_{O_2} \rangle$	$X_{O_2}^{max}$	L_c/L_Z	l_0/L_Z	$\langle Z \rangle$	Z_{st}	Re_{l_0}
0.027	0.035	0.77	0.60	0.008	0.01	96

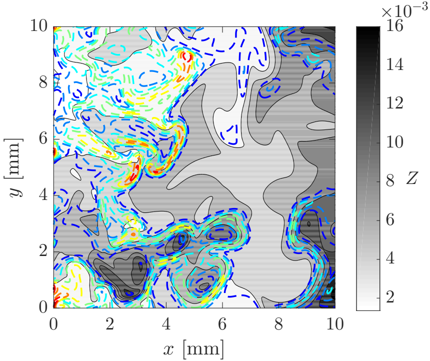
- Moderate temperature increase ($\Delta T \approx 150$K)
- Existence of multiple reaction zones
- Significant reaction zones interactions
- Reactions distributed over a wider region

Morphology of Reaction Zones



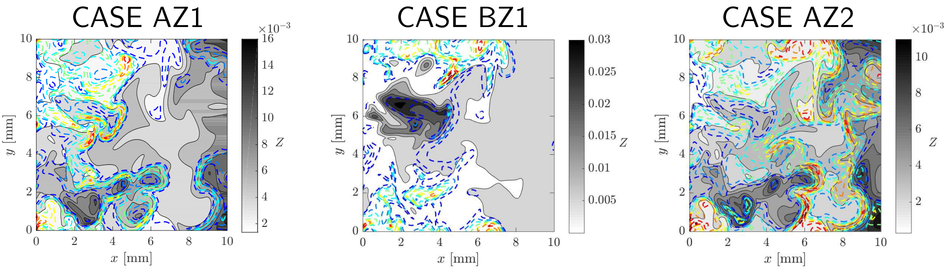
- Convoluted aspect of the reaction zones (heat release)
- Flame-flame interactions → apparent thickening of the reaction zones

Influence of Z on Reaction Zones



- Reaction zones countours (dashed lines) "wrapped" around rich mixture
- Due to higher ignition delay time
- More reactions in lean mixture

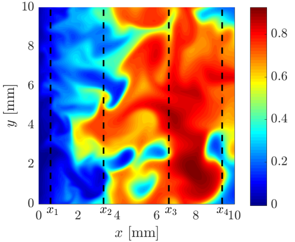
Other DNS Cases



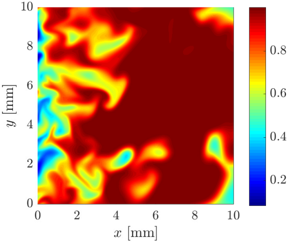
- Rich mixture → low reaction
- Higher dilution → more volumetric reaction

Progress variable in MILD combustion

$$c_T = \frac{T - T^r(Z)}{T^p(Z) - T^r(Z)}$$

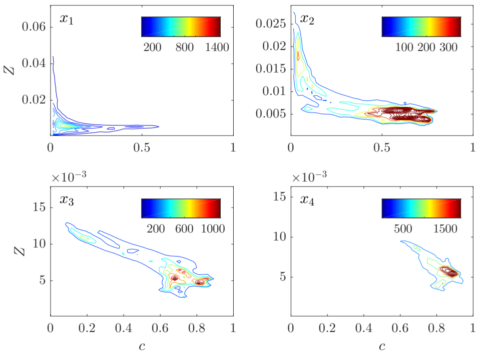


$$c_Y = \frac{Y_{CH_4} - Y^r_{CH_4}(Z)}{Y^p_{CH_4}(Z) - Y^r_{CH_4}(Z)}$$



- c_Y: mostly burned gas → CH_4 quickly consumed by radicals
- c_T: more progressive increase

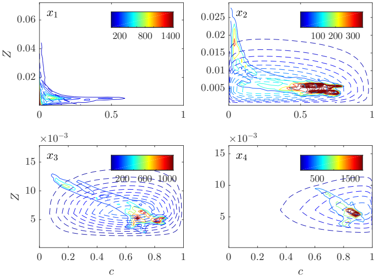
Joint PDF p_{cZ} of c_T and Z



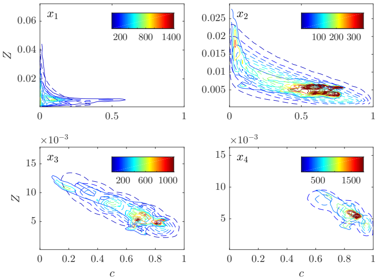
- Distributed and non-bimodal pdf
- Importance of correlation between c_T and Z

Modelling of p_{cZ} with the copula method

Independent β PDF



Correlated PDF (copula method)



- PDF constructed using $\overline{c_T}, \overline{Z}, \overline{c_T''^2}, \overline{Z''^2}$ and $\overline{c_T'' Z''}$
- Substantial improvements by taking into account the covariance
- Qualitative behaviour well capture

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Conclusion

- Preliminary observations from the DNS
  - Convoluted aspect of the reaction zones
  - Apparent thickening by reaction zones interactions
  - Rich mixture $\rightarrow$ lower reaction
  - Higher dilution $\rightarrow$ More volumetric reactions
- Modelling of p_{cZ} using copula method
- Future work:
  - Further study of the structure of reaction zones and interactions
  - Study of flux terms in the joint-PDF equation
  - Modelling of the reaction rate with copula method

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Thank you for your attention.
Questions?

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