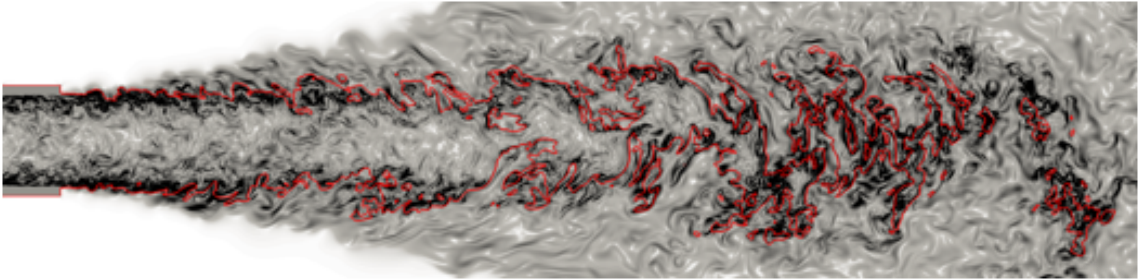
Turbulence-flame interaction in high Reynolds number methane and hydrogen turbulent jet flames



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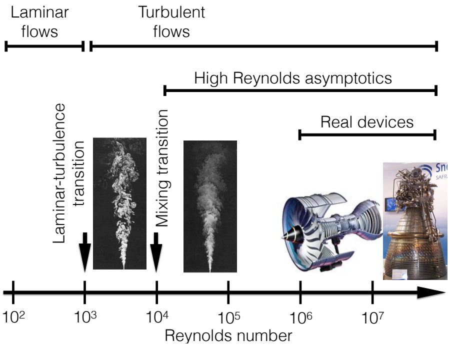
Methane and hydrogen turbulent jet flames

Role of integral scale in methane flames

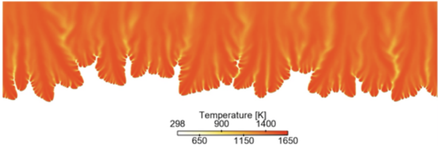
- Lot of effort in achieving high u', not as much for integral scale ℓ.
- Different Re number between DNS/experiments and real devices mostly due to "SIZE" ℓ



Systematic analysis of integral scale effects on turbulent flame speed and turbulence dynamics in flames

Hydrogen combustion and thermo-diffusive instabilities

- Hydrogen important for decarbonization of energy and heat production, energy storage and vector
- Challenging for many reasons
  - High laminar flame speed
  - Flashback and self-ignition
  - **Combustion (thermo-diffusive) instabilities**



Laminar unstable H_2 flame
(Berger, Kleinheinz, Attili, Pitsch PCI 2019)

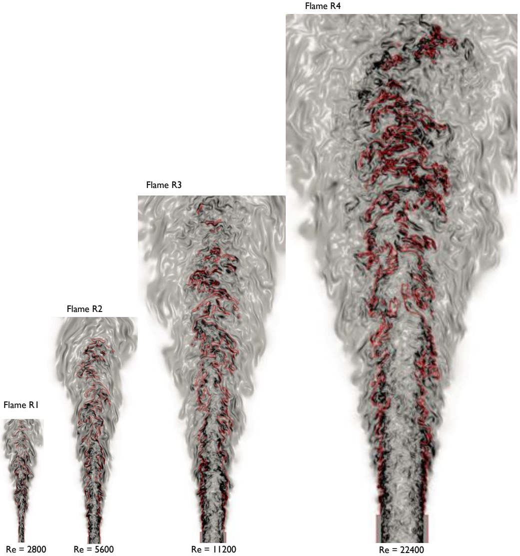
Investigation of thermo-diffusive instability and turbulence interaction

Turbulent methane-air jet flames at increasing Re and constant Ka

- **Configuration** (Luca *et al* PCI 2019, Attili *et al* PCI 2021)
  - Methane-air with $\phi = 0.7$
  - Spatially evolving planar jet, fully developed channel inflow
  - P = 4 atm
  - Pilot with fully burnt product
- **Methods and models** (Attili *et al* CNF 2014)
  - Low Mach, reactive, Navier-Stokes
  - Skeletal mechanism with 16 species (Luca *et al* JPP 2017)
- **Computational Cost (for the largest flame)**
  - 22 Billion grid points, 0.5 Trillion degrees of freedom
  - 80 Millions CPU hours
  - CRAY XC40 supercomputer in KAUST using up to **200K cores**

	R1	R2	R3	R4
Jet Re	2800	5600	11200	22400
Jet U_{bulk}	100 m/s	100 m/s	100 m/s	100 m/s
Slot width H	0.6 mm	1.2 mm	2.4 mm	4.8 mm
Grid points	88 Million	350 Million	2.8 Billion	22 Billion
Karlovitz number	≈40	≈40	≈40	≈40

Goal: assess the effect of the integral scale
(large integral scale usually not achieved in DNS)

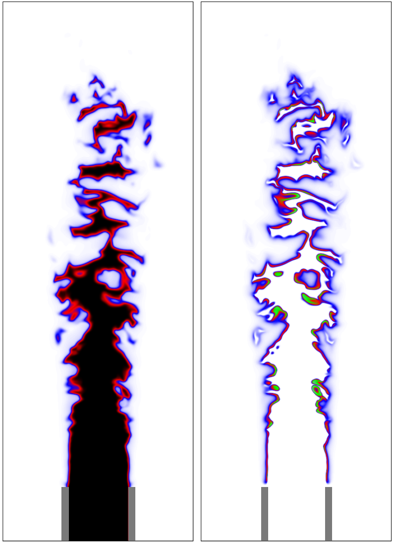


Turbulent hydrogen-air jet flames with thermo-diffusive instabilities

- **Configuration** (Berger, Attili, Pitsch CNF, in preparation)
  - Hydrogen-air with $\phi = 0.4$
  - Spatially evolving planar jet, fully developed channel inflow
  - P = 1 atm
  - Pilot with fully burnt product
- **Methods and models**
  - Low Mach, reactive, Navier-Stokes
  - 9 species hydrogen mechanism
- **Computational Cost**
  - 1 Billion grid points
  - 20 Millions CPU hours
  - SuperMUC-NG supercomputer Leibniz-Rechenzentrum in Munich

	H2 flame
Jet Re	11000
Jet U_{bulk}	24 m/s
Slot width H	8 mm
Grid points	1 Billion
Karlovitz number	≈16

Goal: investigate coupling between turbulence and thermo-diffusive instabilities



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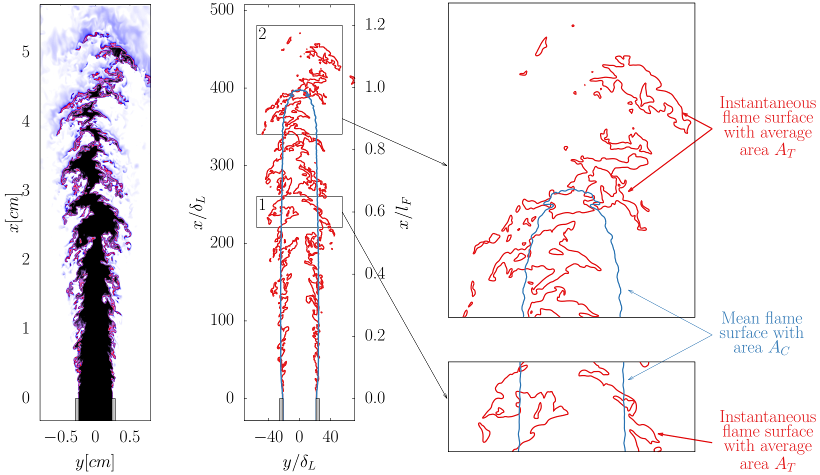


$$S_T(x) = -\frac{\int_{\mathcal{V}} \rho \dot{Y}_{\mathrm{CH}_4} dv}{\rho_u Y_{\mathrm{CH}_4,in} A_C}$$

$$\frac{S_T}{S_L} = I_0 \frac{A_T}{A_C}$$

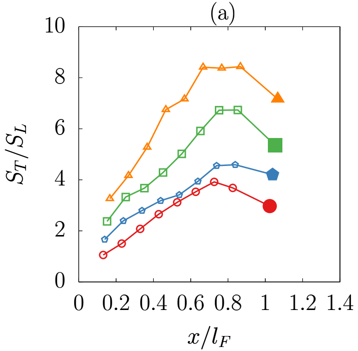
then

$$I_0 = \frac{S_T}{S_L}\frac{A_C}{A_T} = \frac{\Omega^*}{S_L}\frac{1}{A_T}$$

where

$$\Omega^* = -\frac{\int_{\mathcal{V}} \rho \dot{Y}_{\mathrm{CH}_4} dv}{\rho_u Y_{\mathrm{CH}_4,in}}$$

Turbulent flame speed, area ratio and I_0 – methane flames



The turbulent flame speed increases downstream and with Re

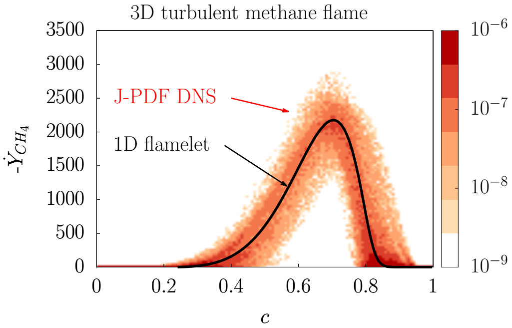
I_0 is larger than 1 and increases downstream and with Re i.e., increases with integral scale

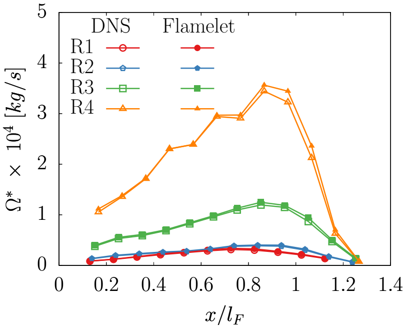
Turbulent flame speed

$$S_T(x) = -\frac{\int_{\mathcal{V}} \rho \dot{Y}_{\mathrm{CH}_4} dv}{\rho_u Y_{\mathrm{CH}_4,in} A_C} \qquad I_0 = \frac{S_T}{S_L}\frac{A_C}{A_T} = \frac{1}{S_L}\frac{\Omega^*}{A_T} \qquad \Omega^* = -\frac{\int_{\mathcal{V}} \rho \dot{Y}_{\mathrm{CH}_4} dv}{\rho_u Y_{\mathrm{CH}_4,in}}$$

Two possible reasons for non-unity I_0:

- variations of $\dot{Y}_{CH_4}$ with respect to 1D planar laminar flame
- variations reaction layer thickness with respect to 1D planar laminar flame





If any, variations of $\dot{Y}_{CH_4}$ have a minor effect in decreasing I_0

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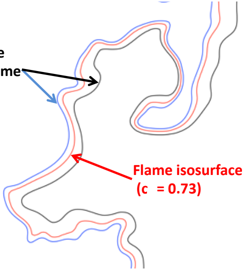
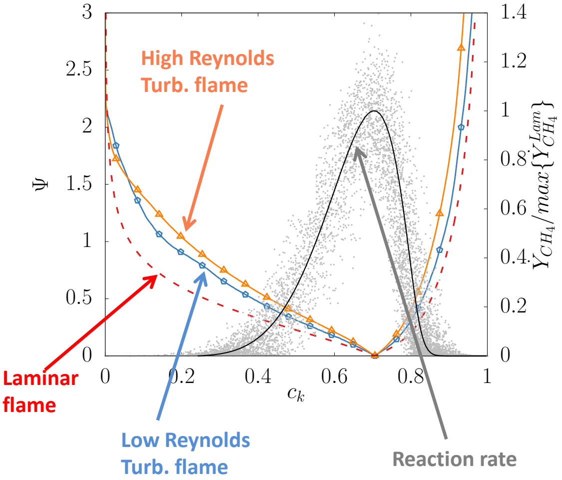
Volume of reactive fluid



Normalized volume between the flame $c = c_0 = 0.73$ and the isosurface c_k.
For $c_k < c_0$:

$$\Psi(c_k) = \frac{1}{\delta_L A_T} \int_{\mathcal{V}} \mathcal{H}(c_0 - c(\mathrm{x}, t))\mathcal{H}(c(\mathrm{x}, t) - c_k) dv$$

(analogously for $c_k > c_0$)



The thickness of the reaction layer is larger compared to the laminar flame and increases with the Reynolds number

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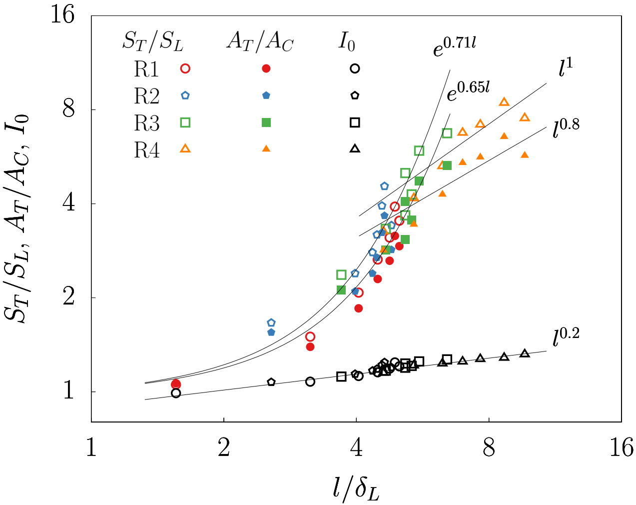
Effect of integral scale



- The turbulent flame speed and flame area
  - For $\ell/\delta_L < 6$: exponential increase
  - For $\ell/\delta_L > 6$: power law

- $I_0 = \frac{S_T}{S_L}\frac{A_C}{A_T}$ grows as $\ell^{0.2}$

- **Note: Ka is constant**

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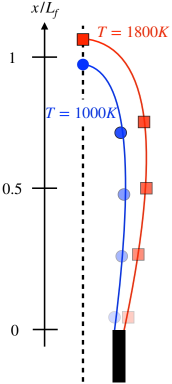
Evolution of turbulence scales across the flame brush

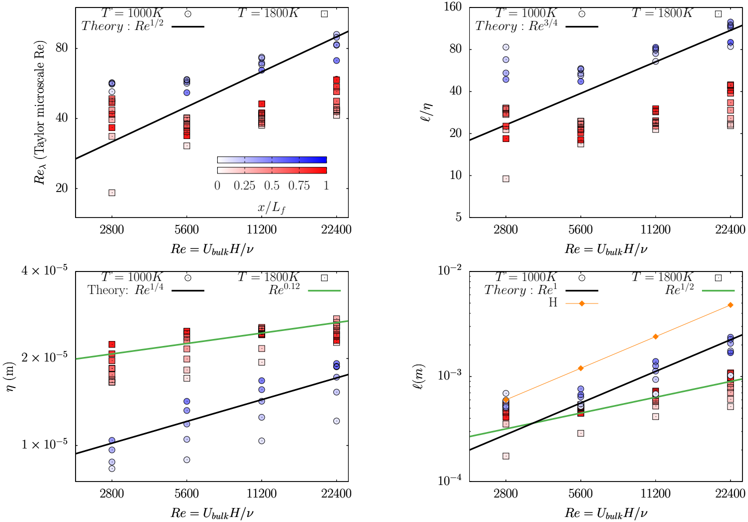


Across the brush:

- Kolmogorov scale η and integral scale ℓ change
- Re decreases
- Ratio ℓ/η decreases: η increases, ℓ decreases

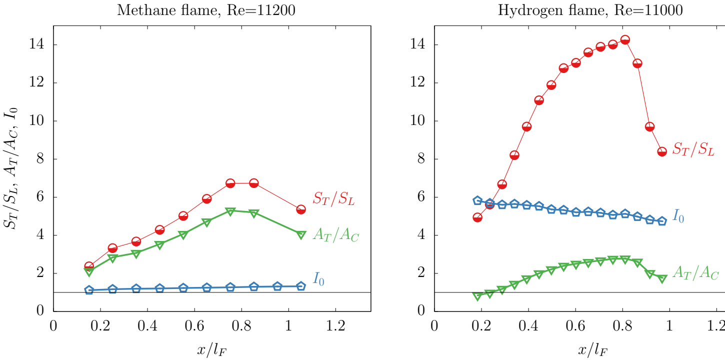
Question:

- Do η and ℓ evolve differently for increasing Re?



For increasing Re, heat release is less effective on small scales and more effective on large scales

Turbulent flame speed in the H2 flame

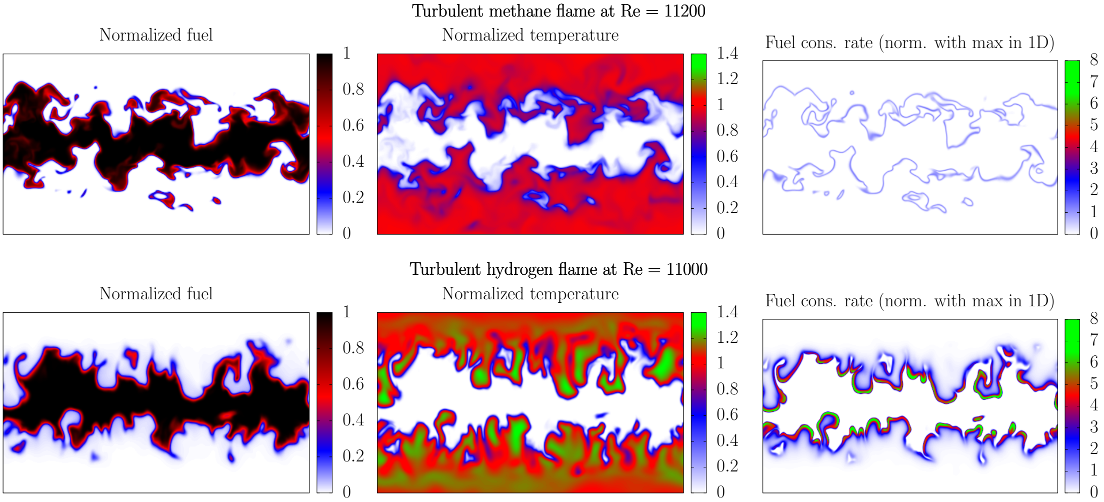


The turbulent flame speed is remarkably high in the H_2 flame

Turbulent flame area plays a relatively small role

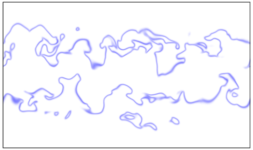
I_0 is extremely high in the H_2 flame (note $Ka = 16$ in the H_2 flame)

Flame visualization and reaction rates

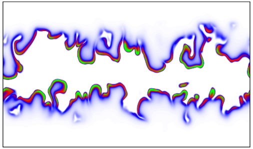


Reaction rates in the hydrogen flame

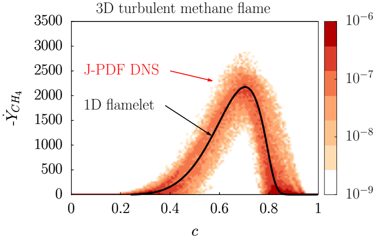
3D turbulent methane flame

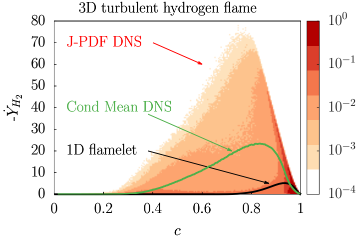


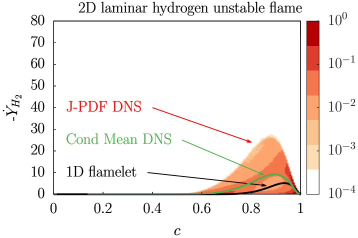
3D turbulent hydrogen flame



2D laminar hydrogen unstable flame



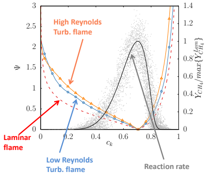




Similar structures in 3D turbulent and 2D laminar hydrogen flames.

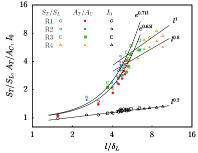
Reaction rate enhancement in turbulent H_2 flame is larger than in H_2 laminar flame.
Synergistic effect of turbulence and thermo-diffusive instabilities.

Conclusions



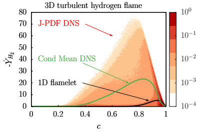
Methane flames:

- Flame surface and turbulent flame speed show power law scaling with integral scale at large Re after exponential growth
- Lack of proportionality between flame area and turbulent flame speed is due to reaction layer thickening
- I_0 increases for increasing Re at constant Ka (increasing integral scale)
- Effect of heat release on turbulence across the brush has more and more effect on large scale for increasing Re



Hydrogen flame:

- Very high I_0 due to thermo-diffusive instabilities strongly enhances turbulent flame speed
- Synergistic effect of turbulence and thermo-diffusive instabilities



Data are available, contact: antonio.attili@ed.ac.uk