Direct Numerical Simulations of Turbulent Stratified Jet Flames

Peter Brearley   Umair Ahmed   Nilanjan Chakraborty

p.brearley@newcastle.ac.uk

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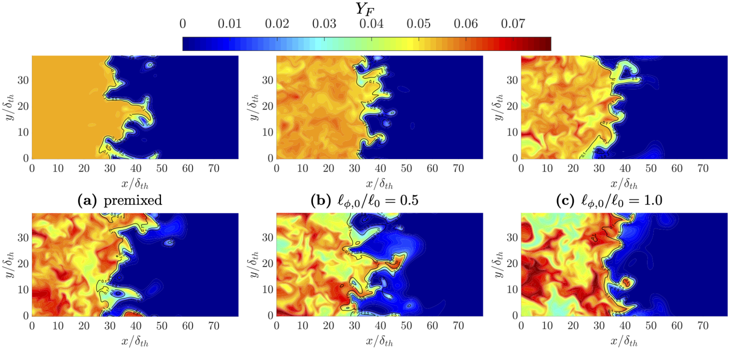
Turbulent stratified mixture combustion

- A limited mixing time is allowed between the unburned reactants such that some premixing takes place but not to the extent of homogeneity.
- Variation in equivalence ratio ϕ across the flame.
- It allows leaner overall mixtures to be used, reducing the burned gas temperature and NO_x emissions.

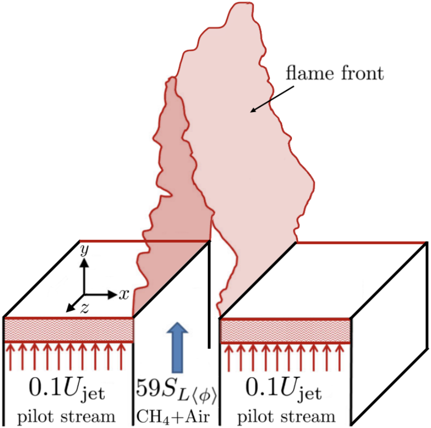


(a) premixed **(b)** $\ell_{\phi,0}/\ell_0 = 0.5$ **(c)** $\ell_{\phi,0}/\ell_0 = 1.0$

(d) $\ell_{\phi,0}/\ell_0 = 1.5$ **(e)** $\ell_{\phi,0}/\ell_0 = 2.0$ **(f)** $\ell_{\phi,0}/\ell_0 = 3.0$

Turbulent slot jet flames

- Direct numerical simulations of a turbulent slot jet flames have been simulated.
- Jet flames are more representative of flames encountered in industrial combustors.
- Cases vary with the alignment of the reaction progress variable gradient with the equivalence ratio gradient, $\nabla c \cdot \nabla \phi$, following the methodology of Richardson & Chen.[1]



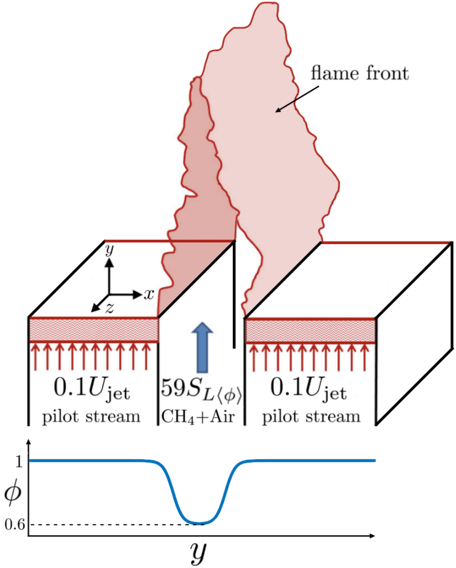
$$c = \frac{\xi Y_{F\infty} - Y_F}{\xi Y_{F\infty} - \max\left\{0, \frac{\xi - \xi_{st}}{1 - \xi_{st}}\right\} Y_{F\infty}}$$

$$\phi = \frac{\xi(1 - \xi_{st})}{\xi_{st}(1 - \xi)}$$

[1] Richardson & Chen (2017). Analysis of turbulent flame propagation in equivalence ratio stratified flow, *Proc. Combust. Inst.* **36**, pp. 1729–1736.

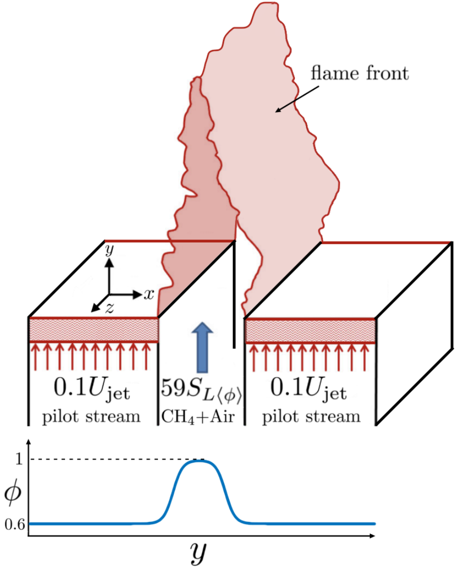
Simulation configuration

- Back-supported flame
  - The mean gradients of equivalence ratio and reaction progress variable are aligned.
  - Initially $\nabla c \cdot \nabla \phi > 0$.
  - $\phi_{\text{coflow}} = 1$ and $\phi_{\text{jet}} = 0.6$
  - The flame is propagating into an increasingly lean fuel-air mixture.



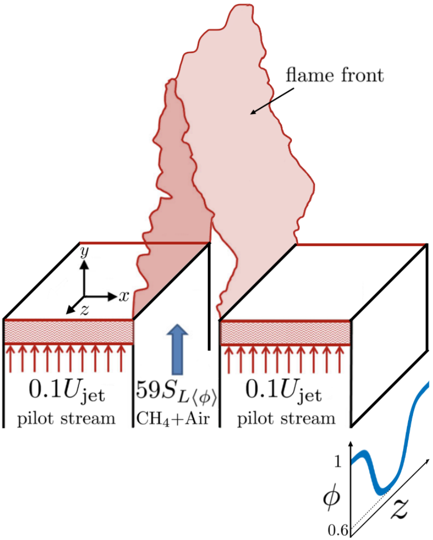
Simulation configuration

- Front-supported flame
  - The mean gradients of equivalence ratio and reaction progress variable are opposed.
  - Initially $\nabla c \cdot \nabla \phi < 0$.
  - $\phi_{\text{coflow}} = 0.6$ and $\phi_{\text{jet}} = 1$
  - The flame is propagating into an increasingly rich fuel-air mixture.



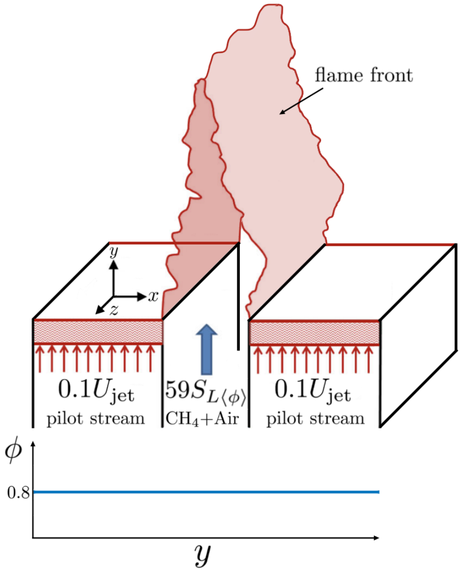
Simulation configuration

- Misaligned scalar gradients
  - The mean gradients of equivalence ratio and reaction progress variable are perpendicular.
  - Initially $\nabla c \cdot \nabla \phi = 0$.
  - $\phi_{\text{jet}} = 0.6$ to 1 and $\phi_{\text{coflow}} = 0.8$.
  - The flame is propagating through a range of equivalence ratio values simultaneously in the z direction.

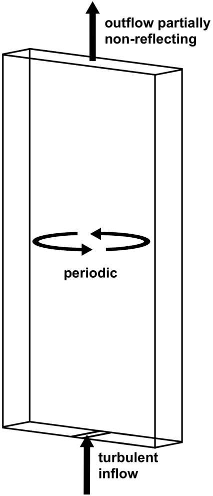


Simulation configuration

- Premixed flame
  - Reference case
  - The flame is propagating through a constant equivalence ratio mixture.
  - $\phi = 0.8$ everywhere, so $\nabla\phi = 0$.

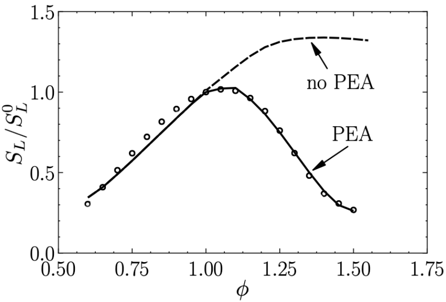


Simulation configuration



- Code used is SENGA+, where the governing equations are solved using a 10th-order finite difference scheme, reducing to 2nd-order and one-sided at non-periodic boundaries.
- Turbulent inflow scans through fully-developed channel flow data.
- Partially non-reflecting outflow specified according to the Navier-Stokes characteristic boundary conditions technique (NSCBC).
- Periodic in the y-z directions.

Thermochemistry



	A (cgs)	β (cgs)	E_a (cal/mol)
$CH_4 + 1.5\ O_2 \Rightarrow CO + 2\ H_2O$	2.00×10^{15}	0.0	35.0×10^3
$CO + 0.5\ O_2 \Rightarrow CO_2$	2.00×10^{9}	0.0	12.0×10^3
$CO_2 \Rightarrow CO + 0.5\ O_2$	8.11×10^{10}	0.0	77.194×10^3

$$k_j = A_j \hat{T}^{\beta_j} \exp\left(\frac{-E_{a,j}}{R\hat{T}}\right)$$

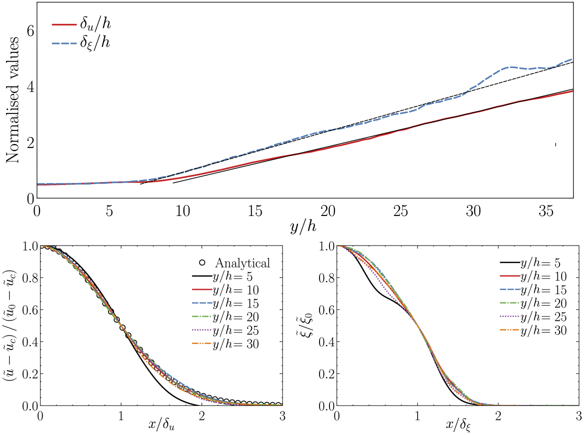
- A two-step chemical mechanism has been used representative of methane-air combustion has been used.[2]
- 5 species solved are CH_4, O_2, CO, CO_2, H_2O.
- A pre-exponential adjustment has been applied applied to rich mixtures.
- It has a low computational cost and ability to accurately estimate the laminar burning velocity across the whole flammability range.

[2] Westbrook & Dryer (1981). Simplified reaction mechanisms for the oxidation of hydrocarbon fuels in flames. *Combust. Sci. Technol.* **27**.

Non-reacting flow validation

- The jet half-width (δ_u, δ_ϕ) is the distance from the centreline to the value halfway between the centreline and coflow values.

- The growth rate of the jet half-width converges to linear growth at $y/h = 10$.
- The evolution of the velocity and scalar from the centreline to coflow values reach similarity also at $y/h = 10$.[3]



[3] Turquand d'Auzay & Chakraborty (2021). The localised forced ignition and early stages of flame development in a turbulent planar jet. *Proc. Combust. Inst.* **38**.

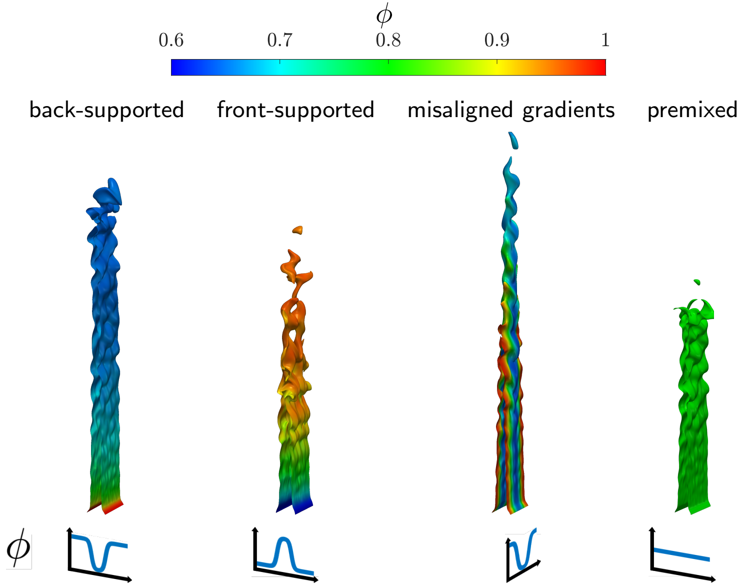
Simulation parameters

Config	$\frac{U_{\text{jet}}}{S_{L\langle\phi\rangle}}$	$\frac{U_{\text{jet}}}{U_{\text{coflow}}}$	$\frac{h}{\delta_{th}}$	Re_{jet}	L/h	Grid size
back-supported	59.1	10	3.0	650	$19\times37\times4.3$	$990\times1920\times225$
front-supported	59.1	10	3.0	650	$19\times37\times4.3$	$990\times1920\times225$
misaligned gradients	59.1	10	3.0	650	$19\times37\times4.3$	$990\times1920\times225$
premixed	59.1	10	3.0	650	$19\times37\times4.3$	$990\times1920\times225$

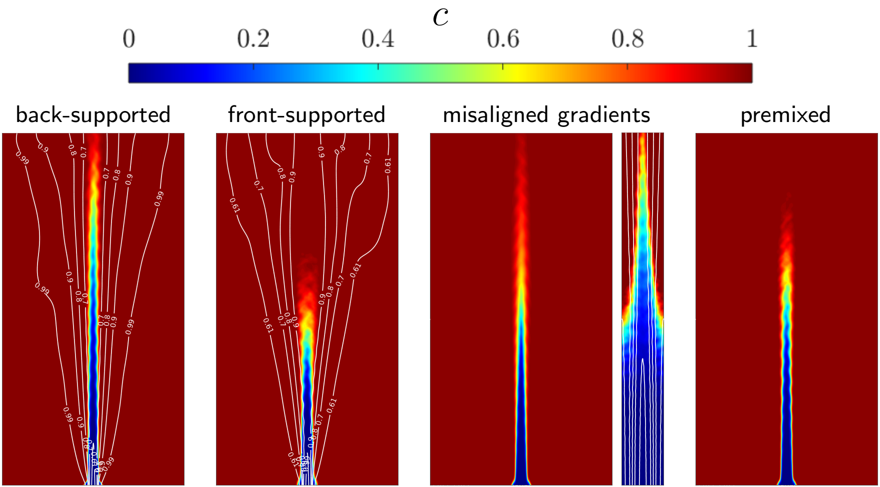
$Re_{\text{jet}} = \rho_0 U_{\text{jet}} h/\mu$

CUs/flowthrough/case: 25,000

3D isosurfaces

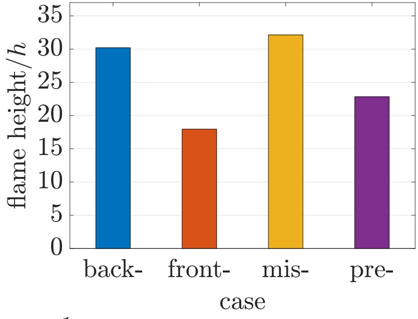


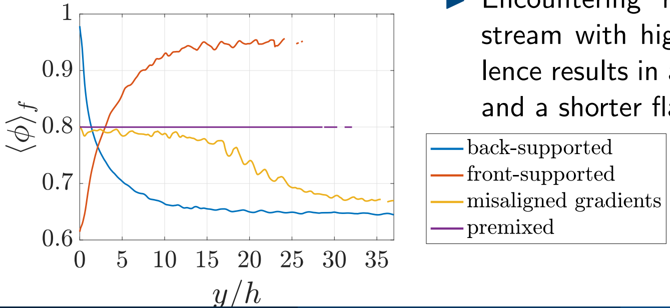
Averaged quantities



- Coloured contours of the reaction progress variable c with the equivalence ratio ϕ contours superimposed.

Flame height and mixture composition

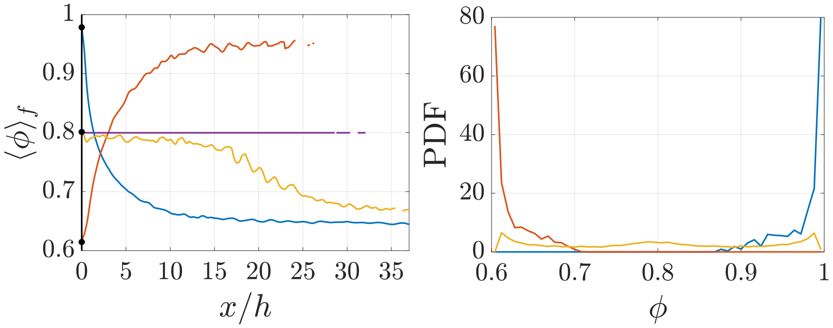




- The equivalence ratio configuration has a large effect on the flame height.
- The average mixture composition within the flame as a function of height supports the observations.
- Encountering richer mixtures upstream with higher levels of turbulence results in a faster burning rate and a shorter flame, and vice versa.

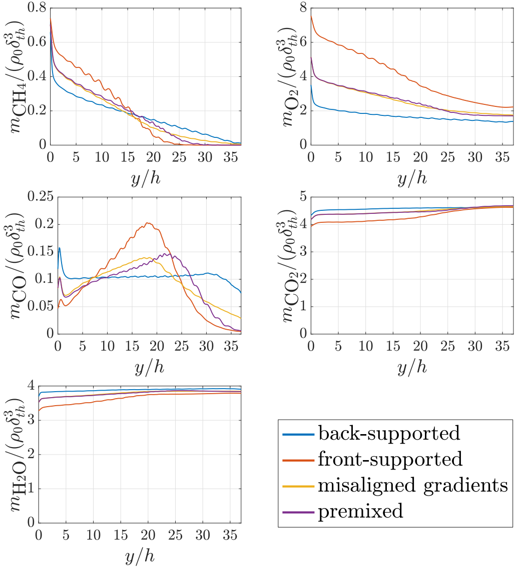
$\langle \phi \rangle_f$ is flame-averaged ϕ

Equivalence ratio PDF within the flame

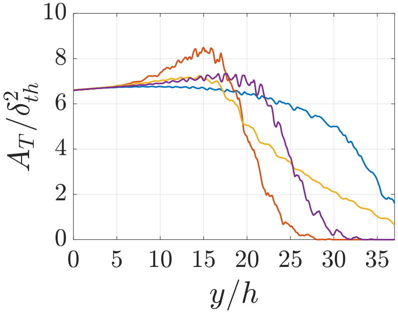


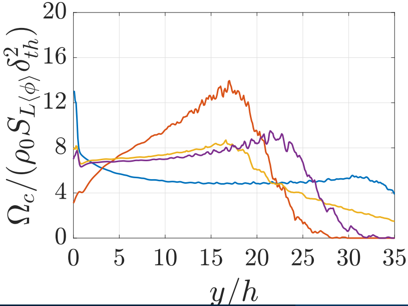
- Variation of the mean equivalence ratio and its PDF within the flame with distance from the inlet.

Evolution of the species mass

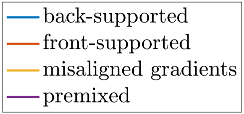


- Evolution of the species mass in the domain as a function of height y.
- ϕ varies from lean to stoichiometric, so the mass of CH_4 goes to zero, and O_2 approaches a non-zero value depending on the burned gas ϕ.
- m_{CO} is the highest in the front-supported case where ϕ and A_T are the highest, then sharply drops to zero because of the lean ϕ in the burned gas.





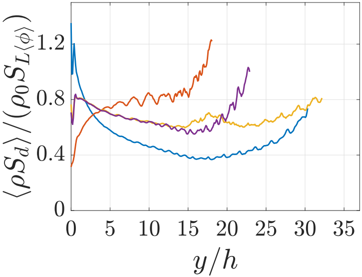
- The mixture composition has a significant effect on the area of the flame.
- Flame-turbulence interaction increases the flame area of the front-supported case when it is encountering the richer mixture, causing the burning rate to increase significantly.

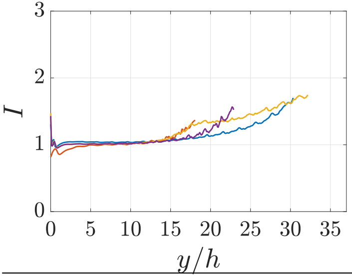


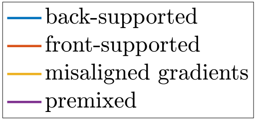
$$A_T = \int_V |\nabla c| \, dV$$

$$\Omega_c = \int_V \dot{\omega}_c \, dV$$

Displacement speed and burning intensity







- The displacement speeds correlate with the local ϕ value, and tends to increase with distance from the inlet regardless of ϕ as the local Reynolds number increases.
- A burning intensity value of 1 indicates that Damköhler's first hypothesis is valid.
- The burning intensity remains at 1 near the inlet but diverges towards the flame tip because of increased curvature.[4]

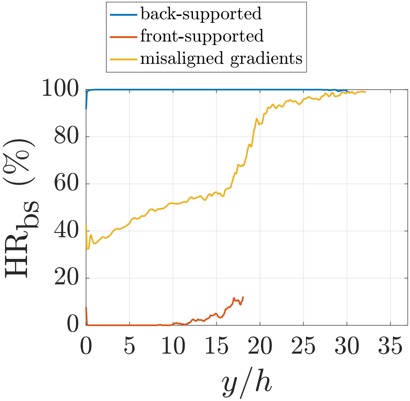
$$S_d = \frac{\dot{\omega}_c + \nabla \cdot (\rho D \nabla c) + A_\xi}{\rho |\nabla c|}$$

$$I = \frac{\int_V \dot{\omega}_c \, dV}{\rho_0 \int_V S_{L(\phi)} |\nabla c| \, dV}$$

[4] Chakraborty et al. (2018). On the validity of Damköhler's first hypothesis in turbulent Bunsen burner flames: A computational analysis. *Proc. Combust. Inst.*

Percentage heat release rate from back-supported burning

$$\mathrm{HR}_{\text{total}} = \int_V H_\phi |\dot{\omega}_F| \, dV$$



- Percentage of the heat release rate arising from the back-supported burning mode.
- Turbulent mixing can alter the mode despite the scalar gradient initialisation.
- The front- and back-supported cases mostly remain as initialised.
- The case with misaligned scalar gradients remains with a 50:50 split while both the richer and leaner mixtures are present.
- As the richer mixture burns away, mostly becomes back-supported.

Conclusions

- Turbulent stratified slot-jets with varying equivalence ratio gradients relative to the reaction progress variable gradient have been simulated.
- Various fundamental flame statistics have been analysed which aid the understanding of flame propagation through equivalence ratio statified mixtures.
- Understanding how the flame interacts with the turbulent stratified mixture is essential to model stratified combustion effectively.

Acknowledgements

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