Stratified Flame Simulations Under Forced Scalar Turbulence

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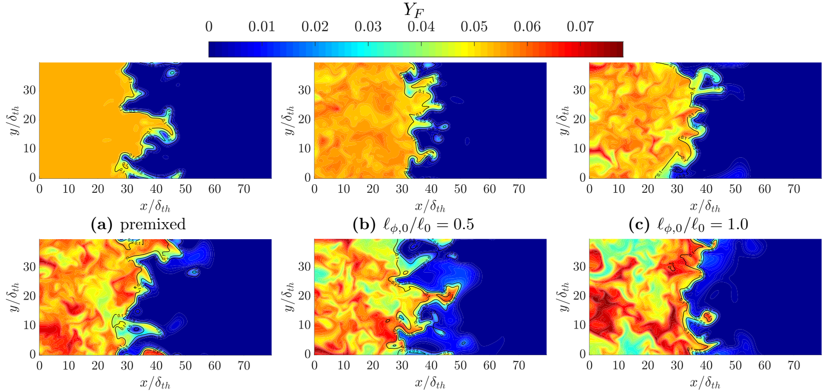
Note: Document must be opened in Adobe Acrobat for animations to play.

What is Stratified Combustion?

- Stratified combustion occurs when the fuel-air mixture is inhomogeneous, but the range of equivalence ratio remains within the flammability limit.
- It allows a leaner unburned mixture to be used, reducing the burned gas temperature and lowering 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)** $\ell_{\phi,0}/\ell_0 = 3.0$

What is Scalar Forcing?

- Scalar forcing aims to maintain the root-mean-square of a fluctuating scalar field e.g. the equivalence ratio

$$\phi = \frac{Y_F/Y_O}{(Y_F/Y_O)_{st}}$$

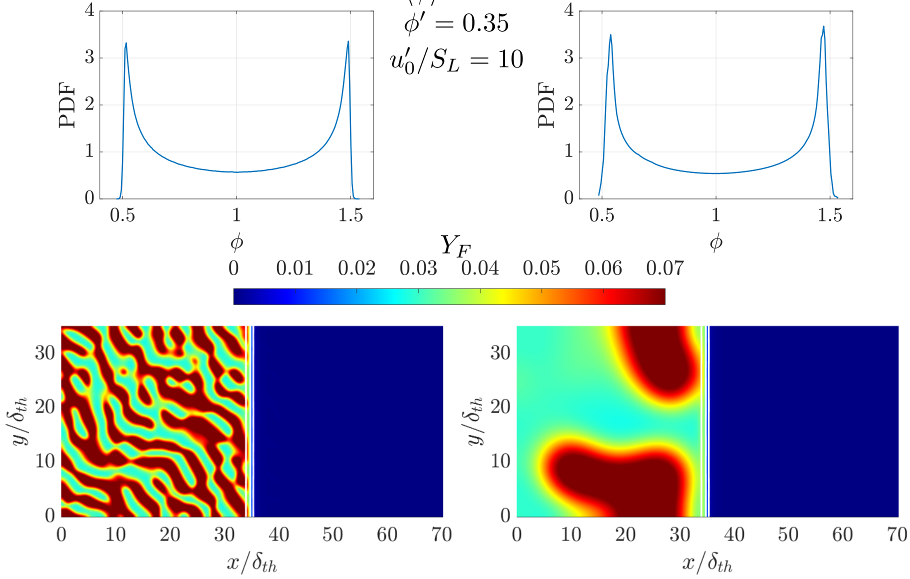
- A source term is added to the scalar transport equation

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho u_k \phi)}{\partial x_k} = \frac{\partial}{\partial x_k}\left(\rho D \frac{\partial \phi}{\partial x_k}\right) + \rho f_\phi,$$

where f_ϕ is the forcing term to be decided

Why is Scalar Forcing Necessary?

$$\langle \phi \rangle = 1.0$$
$$\phi' = 0.35$$
$$u_0'/S_L = 10$$



Mixing Scalar Stratified Flame Simulations

$u'_0/S_{L\langle\phi\rangle}$	$\ell_{\phi,0}/\ell_0$	ℓ_0/δ_{th}	**Da**	**Ka**	$\langle\phi\rangle$	ϕ'_0	**Grid size**
4.0	premixed	3.0	0.750	4.62	1.0	0.35	800×400^2
4.0	0.5	3.0	0.750	4.62	1.0	0.35	800×400^2
4.0	1.0	3.0	0.750	4.62	1.0	0.35	800×400^2
4.0	1.5	3.0	0.750	4.62	1.0	0.35	800×400^2
4.0	3.0	3.0	0.750	4.62	1.0	0.35	800×400^2
8.0	premixed	3.0	0.375	13.1	1.0	0.35	800×400^2
8.0	0.5	3.0	0.375	13.1	1.0	0.35	800×400^2
8.0	1.0	3.0	0.375	13.1	1.0	0.35	800×400^2
8.0	1.5	3.0	0.375	13.1	1.0	0.35	800×400^2
8.0	3.0	3.0	0.375	13.1	1.0	0.35	800×400^2
10	premixed	3.0	0.3	18.3	1.0	0.35	800×400^2
10	0.5	3.0	0.3	18.3	1.0	0.35	800×400^2
10	1.0	3.0	0.3	18.3	1.0	0.35	800×400^2
10	1.5	3.0	0.3	18.3	1.0	0.35	800×400^2
10	3.0	3.0	0.3	18.3	1.0	0.35	800×400^2

Problems With Linear Scalar Forcing Schemes

- Most scalar forcing schemes take inspiration from linear velocity forcing schemes where

$$f_\phi = C\phi' \text{ [1]} \qquad \text{or} \qquad f_\phi = Cu_i' \text{ [2]}$$

- However, turbulent velocity and scalar fields are fundamentally different.
  - The velocity field usually takes on a quasi-Gaussian distribution, whereas scalar fields commonly take on other distributions e.g. bimodal.
  - Scalar fields are often subject to strict bounds e.g. $0 \leq Y_F \leq 1$.
- Linear scalar forcing schemes are not suitable for stratified combustion!

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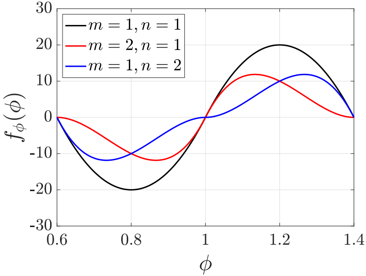
[1] Carroll, P. L., Verma, S., and Blanquart, G. (2013). A novel forcing technique to simulate turbulent mixing in a decaying scalar field, Physics of Fluids 25, 095102.

[2] Overholt, M. R. and Pope, S. B. (1996) Direct numerical simulation of a passive scalar with imposed mean gradient in isotropic turbulence, Physics of Fluids 8, 1328.

Scalar Forcing Scheme Used in This Work

- Daniel et al.[3] proposed a scalar forcing term that can
  - Maintain the scalar root-mean-square fluctuation.
  - Be capable of producing a wide variety of probability density functions (PDFs).
  - Respect the scalars naturally occurring bounds.
- The scalar forcing scheme respects the bounds of the scalar by gradually switching off towards the scalar bounds.



[3] Daniel, D., Livescu, D. and Ryu, J. (2018). Reaction analogy based forcing for incompressible scalar turbulence, Physical Review Fluids 3, 094602.

Scalar Forcing Scheme Used in This Work

- The forcing term

$$f_\phi = \begin{cases} -(\phi_u - \phi_l) mK \left(\frac{\phi_u+\phi_l-2\phi}{\phi_u-\phi_l}\right)^n \left(\frac{\phi-\phi_l}{\phi_u-\phi_l}\right)^m & \text{when } \phi \leq \phi_m \\ +(\phi_u - \phi_l) mK \left(\frac{2\phi-\phi_u-\phi_l}{\phi_u-\phi_l}\right)^n \left(\frac{\phi_u-\phi}{\phi_u-\phi_l}\right)^m & \text{when } \phi > \phi_m \end{cases}$$

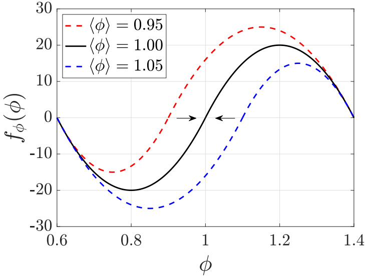
- It was derived by considering a hypothetical chemical reaction that converts a mixed fluid reactant M into its unmixed state E_l or E_u.

$$mM + nE_l \rightarrow (2m+n)E_l \quad \text{when } \phi \leq \phi_m$$
$$mM + nE_u \rightarrow (2m+n)E_u \quad \text{when } \phi > \phi_m$$

[3] Daniel, D., Livescu, D. and Ryu, J. (2018). Reaction analogy based forcing for incompressible scalar turbulence, Physical Review Fluids 3, 094602.

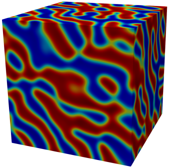
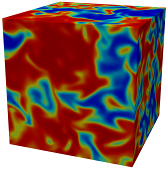
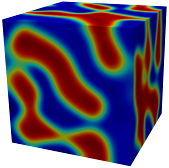
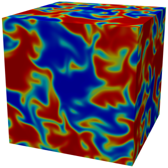
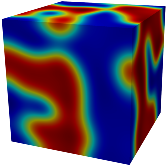
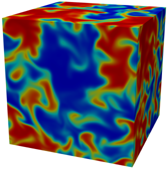
Scalar Forcing Scheme Used in This Work

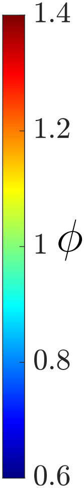
- The forcing scheme by Daniel et al.[3] has been modified to better maintain the mean scalar.
- Otherwise, slight asymmetries in the initial conditions cause the scalar field to be transformed into a uniform state.
- The location where the forcing term crosses the x axis has been modified to be $K_m\langle\phi\rangle$, where K_m is the mean control constant.



[3] Daniel, D., Livescu, D. and Ryu, J. (2018). Reaction analogy based forcing for incompressible scalar turbulence, Physical Review Fluids 3, 094602.

Triply-Periodic Cube Forced Scalar Simulations

ℓ_ϕ/ℓ	Initial conditions		Decaying turbulence
0.5		$\rightarrow$ $18T_{turb}$	
1.0		$\rightarrow$ $18T_{turb}$	
1.5		$\rightarrow$ $18T_{turb}$	



grid: 256^3

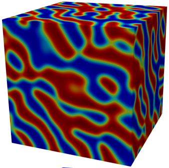
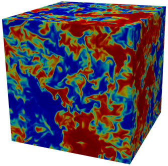
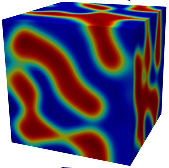
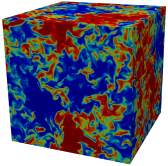
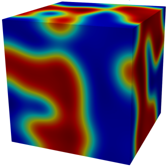
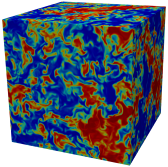
$Re_\lambda = 101$

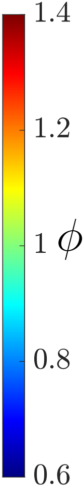
$\langle\phi\rangle = 1.0$

$\phi' = 0.29$

$T_{turb} = \ell/u'$

Triply-Periodic Cube Forced Scalar Simulations

ℓ_ϕ / ℓ	Initial conditions		Lundgren forced turbulence
0.5		$\rightarrow$ $18T_{turb}$	
1.0		$\rightarrow$ $18T_{turb}$	
1.5		$\rightarrow$ $18T_{turb}$	



grid: 256^3

$Re_\lambda = 101$

$\langle \phi \rangle = 1.0$

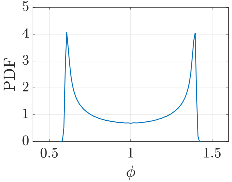
$\phi' = 0.29$

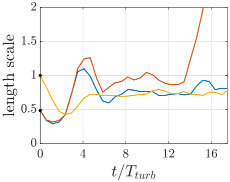
$T_{turb} = \ell / u'$

Triply-Periodic Cube Forced Scalar Simulations

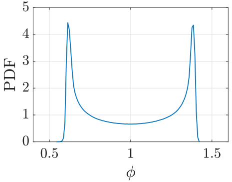
ℓ_ϕ/ℓ	ϕ PDF evolution	Length scale evolution

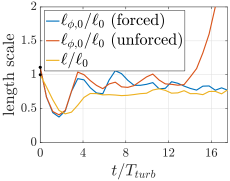
0.5





1.0





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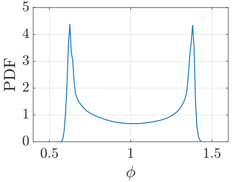
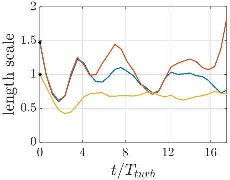




Forced Scalar Stratified Flame Implementation

- Mixture fraction is evaluated from the forced ϕ field using the relation

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

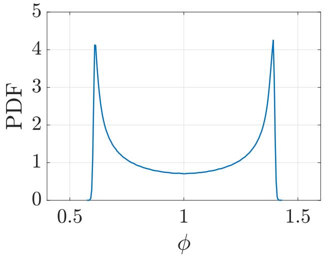
- Then, fuel and oxidiser mass fractions are evaluated by

$$Y_F = \xi Y_{F,\infty} \qquad Y_O = (1-\xi)Y_{O,\infty}$$

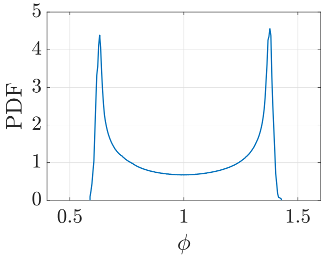
- Scalar forcing is applied only where $c < 0.001$, where c is the combustion progress variable given in stratified flames as

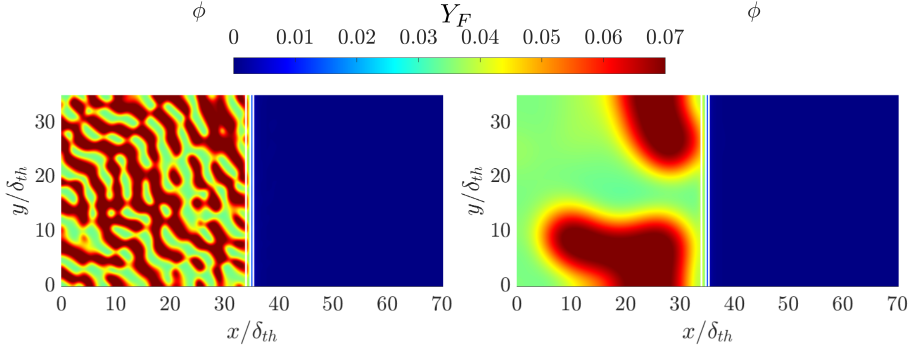
$$c = \frac{\xi Y_{F\infty} - Y_F}{\xi Y_{F\infty} - \max\left[0, \frac{\xi-\xi_{st}}{1-\xi_{st}}\right] Y_{F\infty}}$$

Forced Scalar Reacting Simulations

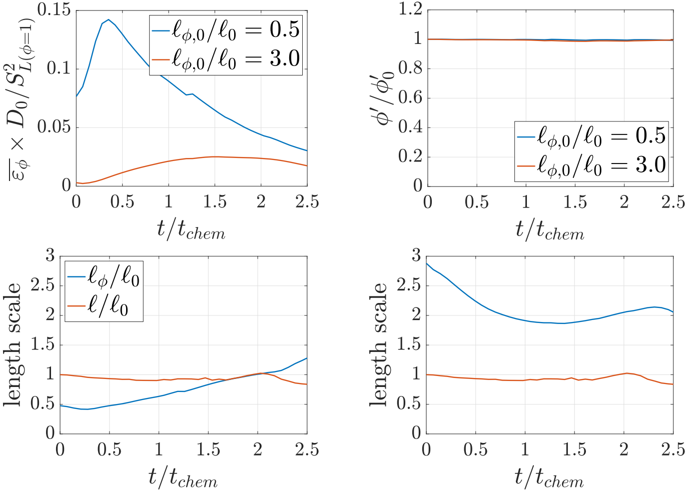


$$\langle\phi\rangle = 1.0$$
$$\phi' = 0.29$$
$$u'/S_L = 5$$





Forced Scalar Reacting Simulations



$\ell_{\phi,0}/\ell_0 = 0.5$ $\ell_{\phi,0}/\ell_0 = 3.0$

Future Direction

- Demonstrate that the scalar forcing scheme does not artificially modify the physics of the turbulent stratified flame.
- Use the newly developed research tool to investigate the the effects of highly stratified unburned mixtures on turbulent flames.
- Lundgren forcing will be developed into bandwidth filtered forcing[4].
- The scalar forcing scheme will be used with more detailed chemical mechanisms.

Acknowledgements

I am grateful to ARCHER, Cirrus, (kAU: 10,000, code: SENGA+) and Rocket HPC services for computational support, and to EPSRC for financial support.

[4] Klein, M., Chakraborty, N., and Ketterl, S. (2017). A comparison of strategies for direct numerical simulation of turbulence chemistry interaction in generic planar turbulent premixed flames, Flow, Turbulence and Combustion 99, pp. 955–971.