Scalar Forcing Methodology for Direct Numerical Simulations of Turbulent Stratified Mixture Combustion

Peter Brearley   Umair Ahmed   Nilanjan Chakraborty

p.brearley@newcastle.ac.uk

UKCTRF Conference
30th March 2021

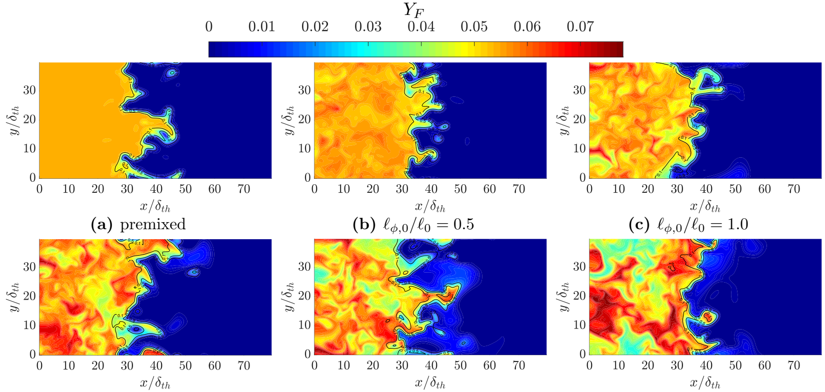
Newcastle University

UK CTRF UK CONSORTIUM ON TURBULENT REACTING FLOWS 2014 - 2023

archer

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

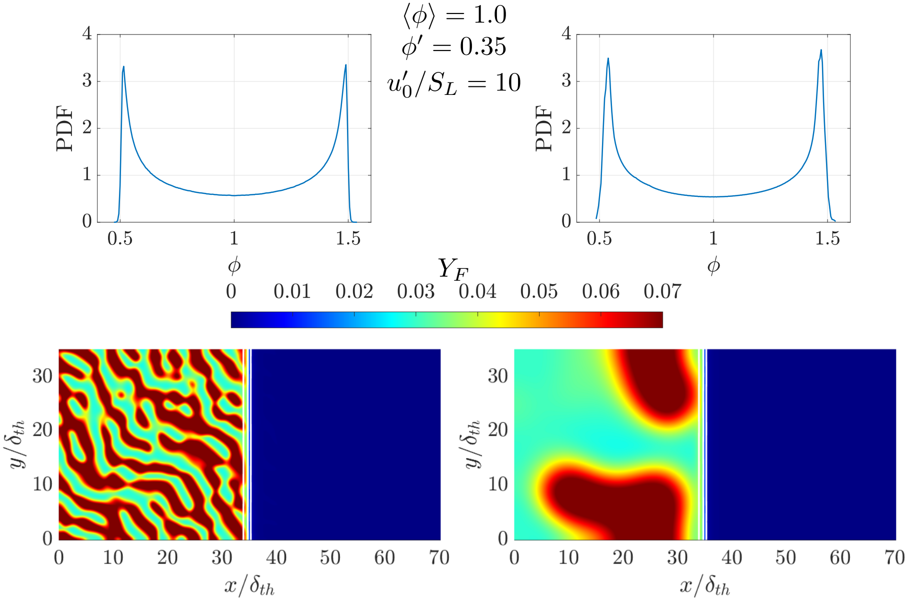
What is Scalar Forcing?

- Scalar forcing aims to maintain the root-mean-square of a fluctuating scalar field ψ by including a source term in its transport equation

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

- In stratified combustion, this scalar could be the mixture fraction ξ or equivalence ratio ϕ
- Choosing an appropriate f_ψ term for use in stratified combustion is the focus of this study.

Why is Scalar Forcing Necessary?



Mixing Scalar Stratified Flame Simulations

$u'_0/S_{L\langle\phi\rangle}$	$\ell_{\xi,0}/\ell_0$	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	2.0	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	2.0	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	2.0	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

[1] Brearley, P., Ahmed, U., and Chakraborty, N. (2013). Physics of Fluids 32, 125111.

Problems With Linear Scalar Forcing Schemes

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

$$f_\psi = C\psi' \text{ [2]} \qquad \text{or} \qquad f_\psi = Cu_i' \text{ [3]}$$

- 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 might not be appropriate for stratified combustion.

[2] Carroll, P. L., Verma, S., and Blanquart, G. (2013). Physics of Fluids 25, 095102.
[3] Overholt, M. R. and Pope, S. B. (1996). Physics of Fluids 8, 1328.

Scalar Forcing Scheme Used in This Work

- Daniel et al.[4] 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.
- The forcing term is given by

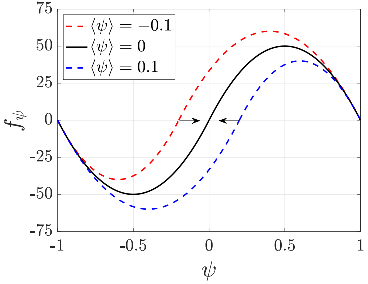
$$f_\psi = \begin{cases} -(\psi_u - \psi_l) mK \left(\frac{\psi_u + \psi_l - 2\psi}{\psi_u - \psi_l}\right)^n \left(\frac{\psi - \psi_l}{\psi_u - \psi_l}\right)^m & \text{when } \psi \le \psi_m \\ +(\psi_u - \psi_l) mK \left(\frac{2\psi - \psi_u - \psi_l}{\psi_u - \psi_l}\right)^n \left(\frac{\psi_u - \psi}{\psi_u - \psi_l}\right)^m & \text{when } \psi > \psi_m \end{cases}$$

- It was derived by considering a hypothetical chemical reaction that converts a mixed fluid reactant into one of its two unmixed states.

[4] Daniel, D., Livescu, D. and Ryu, J. (2018). Physical Review Fluids 3, 094602.

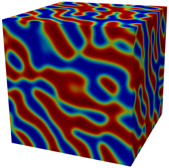
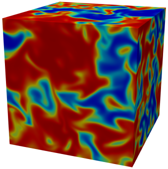
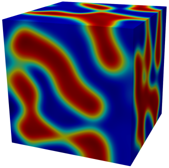
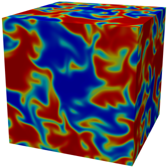
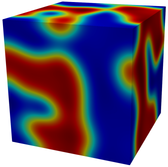
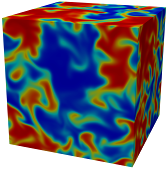
Scalar Forcing Scheme Used in This Work

- The forcing scheme by Daniel et al.[4] 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 $K_m\langle\psi\rangle$, where K_m is the mean control constant.



[4] Daniel, D., Livescu, D. and Ryu, J. (2018). Physical Review Fluids 3, 094602.

Periodic Cube Bimodal Forced Scalar Simulations

ℓ_ψ/ℓ	Initial conditions		Decaying velocity field
0.5		$\rightarrow$ $18T_{turb}$	
1.0		$\rightarrow$ $18T_{turb}$	
1.5		$\rightarrow$ $18T_{turb}$	

grid: 256^3

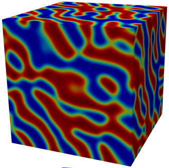
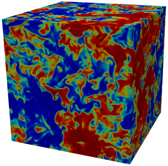
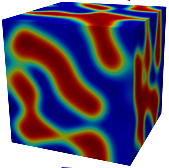
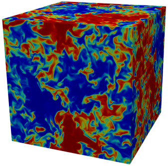
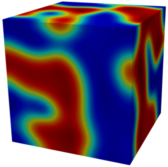
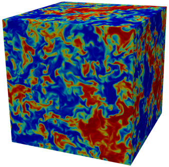
$Re_\lambda = 101$

$\langle\psi\rangle = 1.0$

$\psi' = 0.29$

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

Periodic Cube Bimodal Forced Scalar Simulations

ℓ_ψ/ℓ	Initial conditions		Lundgren forced velocity field
0.5		$\rightarrow$ $18T_{turb}$	
1.0		$\rightarrow$ $18T_{turb}$	
1.5		$\rightarrow$ $18T_{turb}$	

grid: 256^3

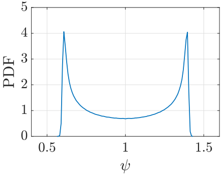
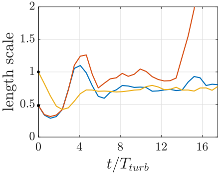
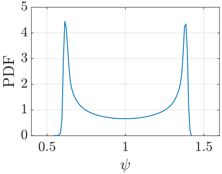
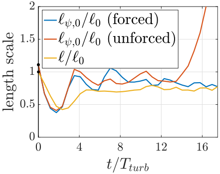
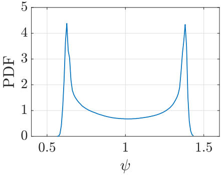
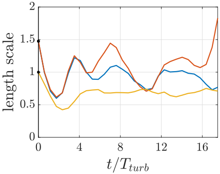
$Re_\lambda = 101$

$\langle\psi\rangle = 1.0$

$\psi' = 0.29$

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

Periodic Cube Bimodal Forced Scalar Simulations

ℓ_ψ/ℓ	ψ PDF evolution	Length scale evolution
0.5		
1.0		
1.5		

Lundgren forcing

grid: 256^3

$Re_\lambda = 101$

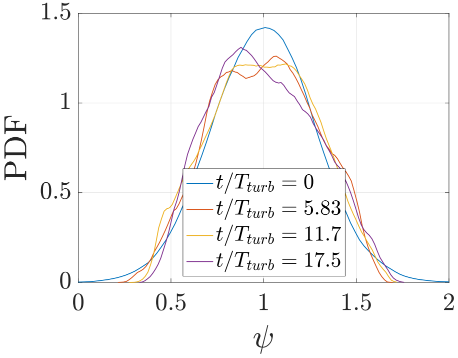
$\langle\psi\rangle = 1.0$

$\psi' = 0.29$

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

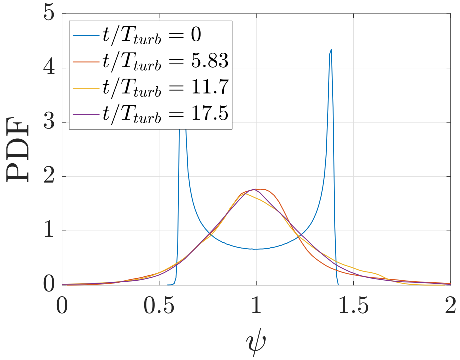
Periodic Cube Gaussian Forced Scalar Simulations

- The scalar forcing scheme can maintain any symmetric scalar distribution in the transition between Gaussian and bimodal.
- The figure below shows the forcing scheme maintaining a Gaussian distribution.



Linear Scalar Forcing with Bimodal Scalar Distributions

- Linear scalar forcing[5] can maintain Gaussian scalar distributions very effectively, but cannot maintain other distributions.



[5] Carroll, P. L., Verma, S. and Blanquart, G. (2013). Phys. Fluids 25, 095102

Forced Scalar Stratified Flame Implementation

- At the end of each timestep, fuel and oxidiser mass fractions are evaluated by

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

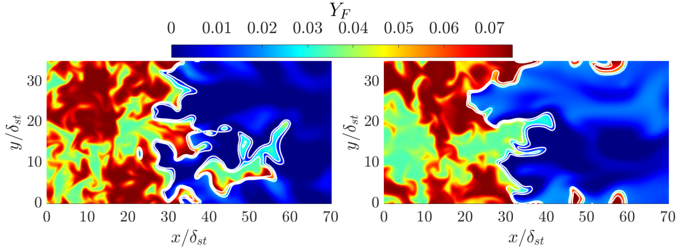
- Scalar forcing is applied only where $c < 0.001$, where c is the combustion progress variable given in stratified flames as

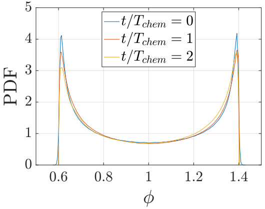
$$c = \frac{\xi Y_{F\infty} - Y_F}{\xi Y_{F\infty} - \max\left[0, \frac{\xi - \xi_{st}}{1-\xi_{st}}\right] Y_{F\infty}}$$

- Modified-bandwidth filtered linear velocity forcing scheme is used that can maintain the turbulence length scale as well as the rms.[6]

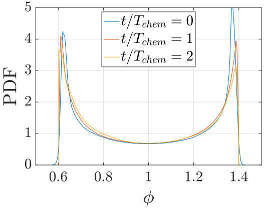
[6] Klein, M., Chakraborty, N., and Ketterl, S. (2017). Flow, Turbulence and Combustion 99, pp. 955–971.

Forced Scalar Reacting Simulations





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



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

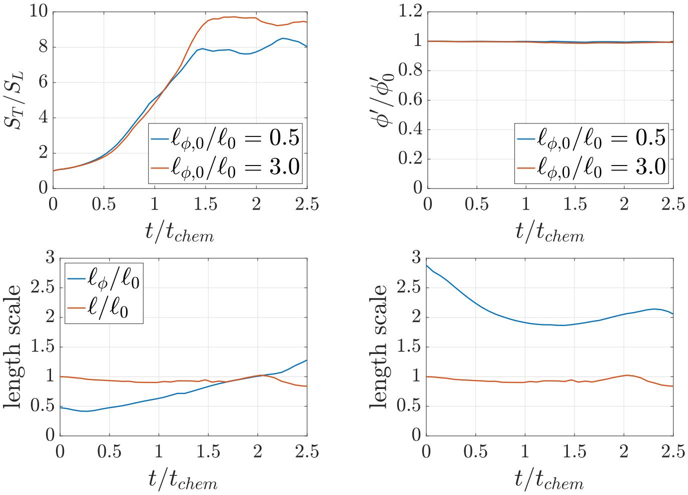
$\langle\phi\rangle = 1.0$

$\phi' = 0.29$

$u'/S_L = 5$

$t/T_{chem} = 2$

Forced Scalar Reacting Simulations



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

Future Direction

- Further 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.
- The scalar forcing scheme will be used with more detailed chemical mechanisms.

Acknowledgements

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