A priori assessment of combustion models for MILD combustion using Direct Numerical Simulation data

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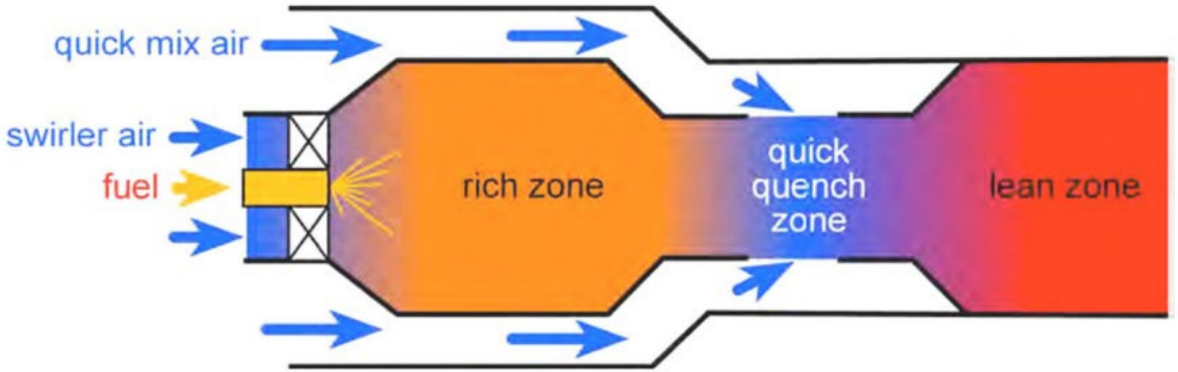
Introduction

Low Emissions Combustion Techniques:

- Rich burn – quick quench– lean burn (RQL) combustion
- Water and steam injection
- Lean-premixed (LP) combustion

Thus, there is a need of a simple combustion technique that can simultaneously improve efficiency, reduce emissions and enhance the combustion stabilities

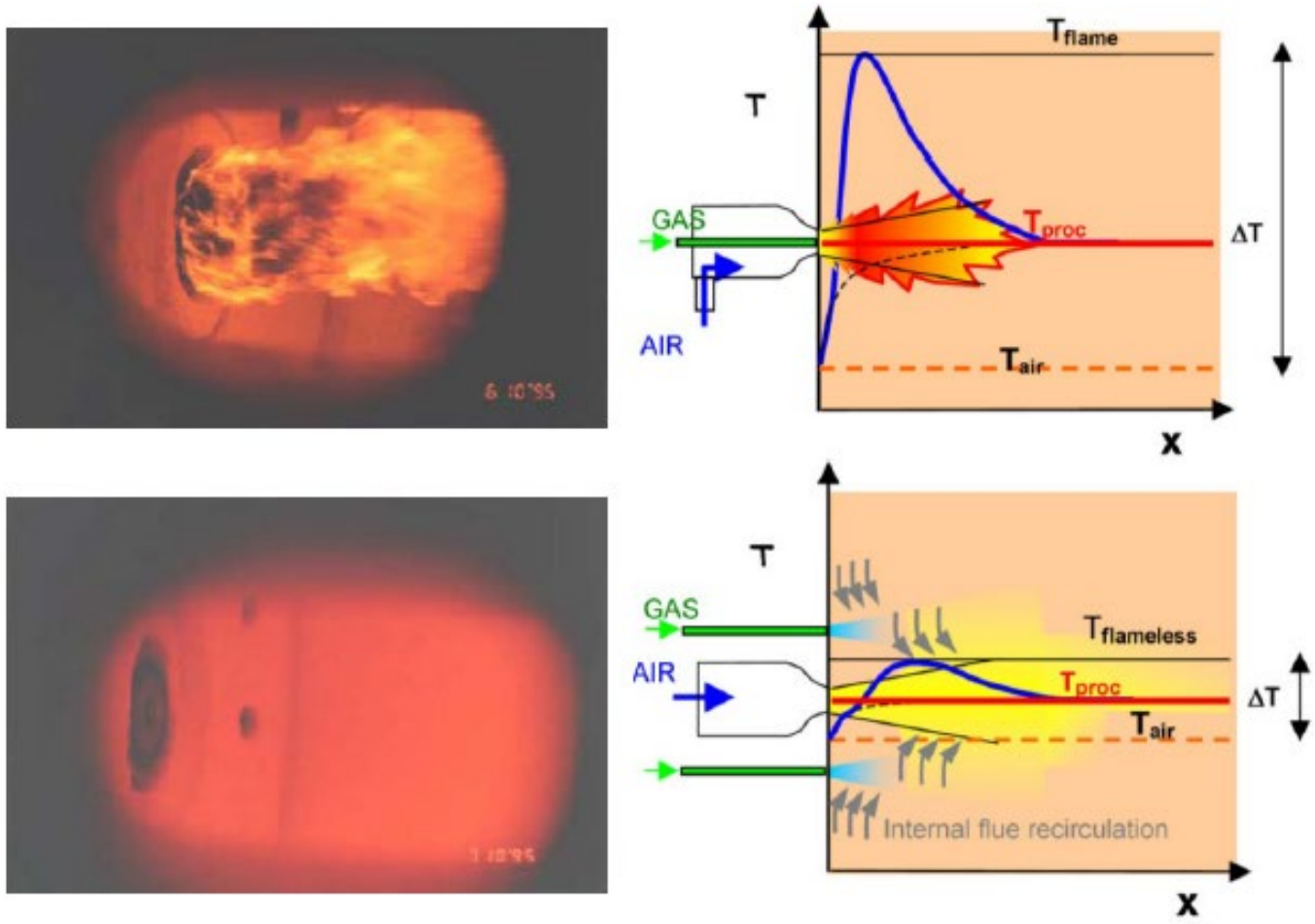


RQL combustor [1]

[1] Benini, E. (Ed.). (2013). Progress in gas turbine performance.

Moderate or Intense Low-Oxygen Dilution (MILD) Combustion

- MILD combustion was discovered in 1989 during trials aimed for NO_x reduction.
- No flame could be detected in the combustion chamber.
- Compared to LP , MILD combustion improves combustion stability, provides uniform temperature distribution and eliminates the need of using a pilot for stabilizing the flame.
- $T_o > T_{ign}$ and $\Delta T < T_{ign}$



MILD (bottom) vs. conventional (top) combustion [1]

[1] Benini, E. (Ed.). (2013). Progress in gas turbine performance.

Motivations and objectives

- Previous Reynolds Averaged Navier-Stokes (RANS) and large eddy simulation (LES) investigations of MILD combustion revealed discrepancies with experimental data in terms of the peak temperature and minor species.

- Despite its advantages, MILD combustion is still not well understood, and modelling MILD combustion is a challenging task.

- To carry out an a priori assessment of different mean reaction rate and scalar dissipation rate (SDR) closures in the context of RANS simulations by using Direct numerical simulation (DNS) data of homogenous mixture MILD combustion of methane (CH_4).

Numerical Implementation

- The simulations have been conducted using a 3D compressible DNS code SENGA2 [1].
- Spatial derivatives are evaluated using a 10^{th}-order central difference scheme for the internal grid points which gradually drops to a 4^{th}-order one-sided scheme at the non-periodic boundaries.
- The time advancement has been achieved by an explicit 4^{th}-order Runge–Kutta scheme
- A skeletal mechanism of CH4–air combustion involving 16 species and 25 reactions [2].
- Boundary conditions are specified using the NSCBC technique. The left x-direction has a turbulent inflow with specified density, species, and velocity boundary condition while the right x-direction has a partially non-reflective outflow boundary condition.
- The grid spacing ensures that the thermal flame thickness is resolved with 12 grid points and the Kolmogorov length scale remains garter than the grid size.

[1] Cant, R.S. Technical Report CUED/A–THERMO/TR67; Cambridge University Engineering Department: Cambridge, UK, 2012.
[2] Smooke, M.D.; Giovangigli, V. Premixed and Nonpremixed Test Flame Results; Springer: Berlin/Heidelberg, Germany, 1991; pp. 29–47.

Homogenous mixture MILD combustion simulation parameters

Thermochemical conditions for the 1D unstretched laminar premixed flames

Dilution	X_{O_2}	X_{CO_2}	X_{H_2O}	X_{CH4}	X_{N_2}	$S_L(m/s)$	$\delta_{th}(mm)$	$T_0(K)$	Φ
4.8% O_2	0.048	0.061	0.121	0.019	0.751	3.20	0.62	1500	0.8
3.5% O_2	0.035	0.066	0.132	0.014	0.753	2.30	0.80	1500	0.8

$\delta_{th} = (T_{ad} - T_0)/max|\nabla T|_{Laminar}$ is the thermal flame thickness

T_0 is the reactant tempreature

T_{ad} is the adiabatic flame tempreature

- Each case is simulated at 2 turbulence intensities resulting in total of 4 cases.

Turbulence parameters for SET A and B

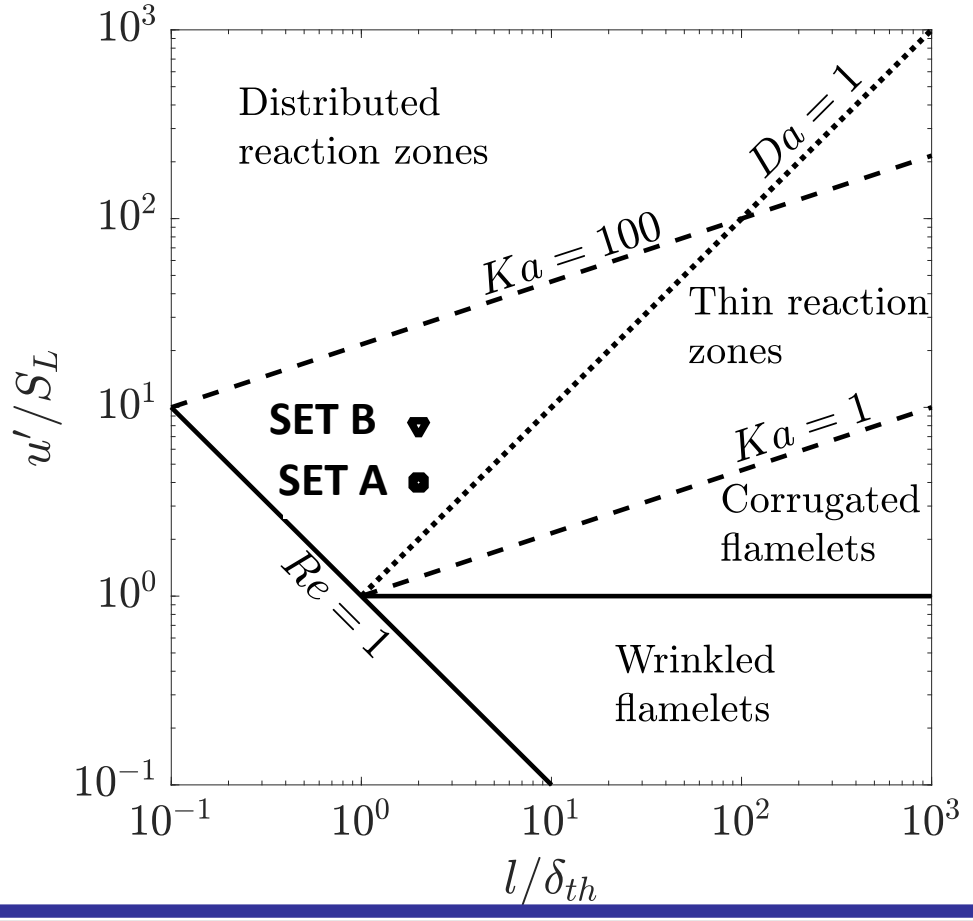
SET	u'/S_L	l/δ_{th}	Da	Ka
A	4.0	2.5	0.62	5.06
B	8.0	2.5	0.31	14.31

$$Da = l S_L/u' \delta_{th}$$

$$Ka = (u'/S_L)^{3/2}(l/\delta_{th})^{-1/2}$$

MILD combustion cases on the regime diagram

- The investigated cases are in the same location on the Borghi–Peters diagram [1]
- All the cases considered here nominally represent combustion within the thin reaction zones regime [1]



[1] N. Peters, Turbulent Combustion, 1st ed. (Cambridge University Press, 2000).

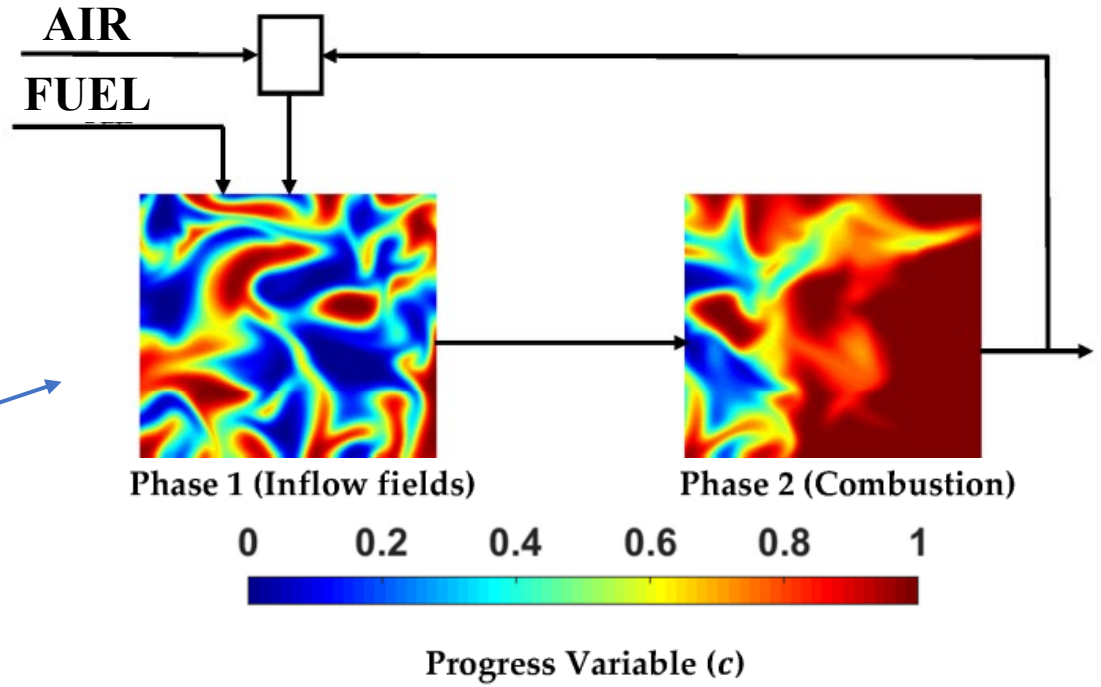
Homogenous mixture MILD combustion initialisation

- The homogenous mixture MILD combustion is initialized following the methodology proposed by Minamoto et al. [1]
- The first phase corresponds to the mixing of the products of combustion with the reactant mixture by recirculation. It acts as the initial conditions as well as the inflow fields for second phase.
- The second phase simulates MILD combustion.

1) Homogenous isotropic turbulence is generated using a well-known pseudo-spectral method.

2) Thermochemical conditions are used to simulate the 1D laminar premixed flame. The laminar solution is parameterised as a function of c. A bimodal distribution of c is specified and the scalar field is initialised using the laminar flame parameterisation.

3) The generated bimodal fields are then allowed to evolve with turbulence for about 1 turnover time.

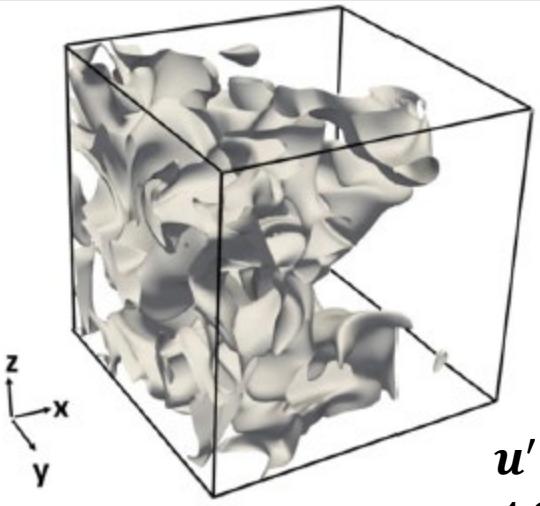


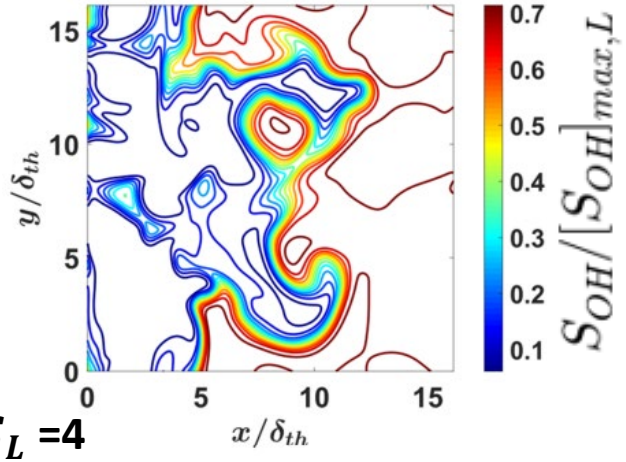
$$c = \frac{Y_\alpha - Y_{\alpha R}}{Y_{\alpha P} - Y_{\alpha R}}$$ Y_α is the mass fraction of species α

R : unburned reactants and P: fully burned products

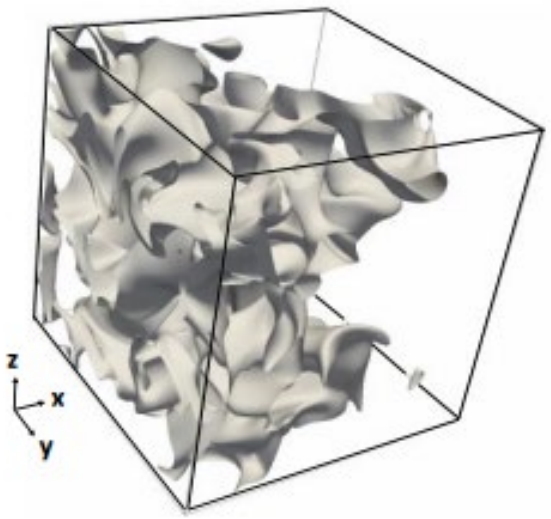
MILD combustion reaction zone

- MILD combustion shows interaction of reaction zones
- The extent of the interaction depends more on the dilution than the turbulence.
- **OH-PLIF** signal ($S_{OH} \propto X_{OH} T^{-\beta}$ where $-2.6 \leq \beta \leq 1$) [1] reveals thick reaction zone in MILD combustion



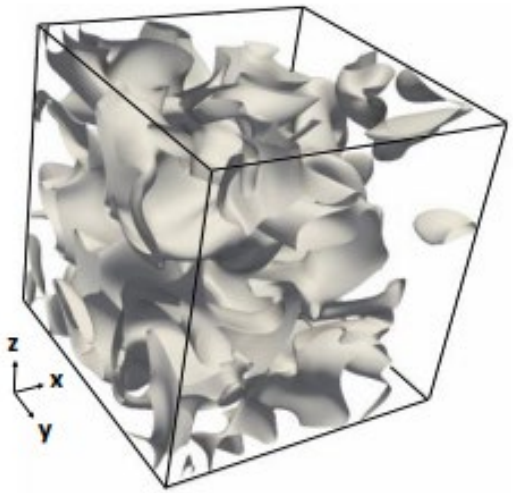


u'/S_L =4
4.8 % O_2

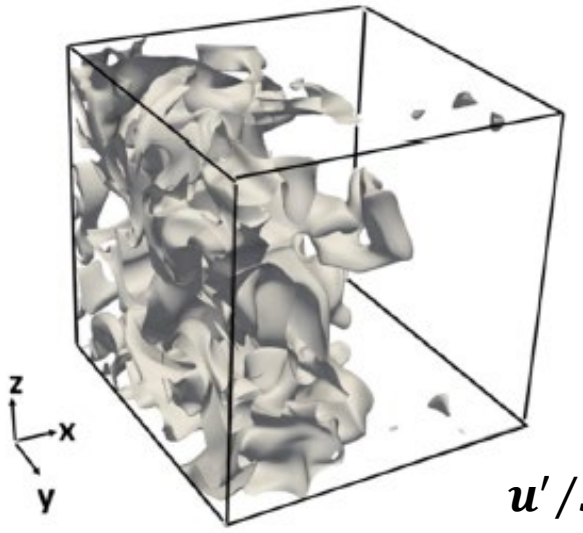


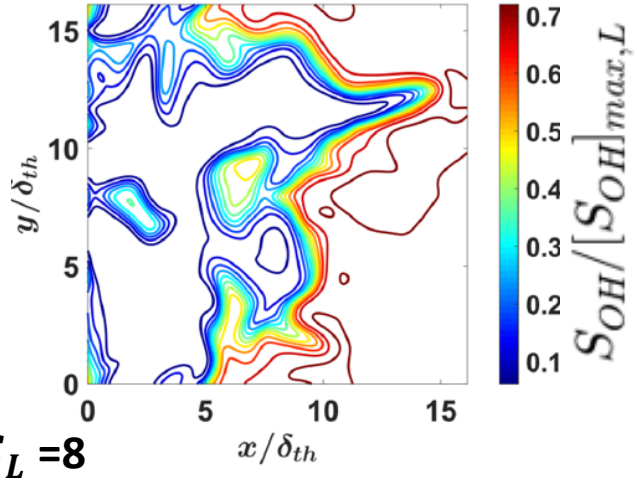
4.8 % O_2

u'/S_L = 4.0



3.5 % O_2





u'/S_L =8
4.8 % O_2

c = 0.8 i*sosurface*

OH-PLIF signal S_{OH}

[1] Paul, P.H.; Najm, H.N. Planar laser-induced fluorescence imaging of flame heat release rate. Proc. Combust. Inst. 1998, 27, 43–50.

Combustion modelling approaches

- Assessing the use of the presumed PDF modelling approach.
- Assessing different algebraic SDR closures for the presumed pdf modelling approach.
- Assessing modelling of the mean reaction rate using the modified eddy breakup (EBU) model and the eddy dissipation concept (EDC).
- Assessing modelling of the mean reaction rate using the flame surface density (FSD) and SDR closures.

Modelling by Presumed PDF

- In the context of tabulated chemistry, the presumed pdf approach provides a closure for $\overline{\dot{\omega}_c}$ by integrating tabulated values of $\dot{\omega}_c$ with the presumed PDF:

$$\overline{\dot{\omega}_c} = \int_0^1 \dot{\omega}_c\,(c) P(c) dc$$

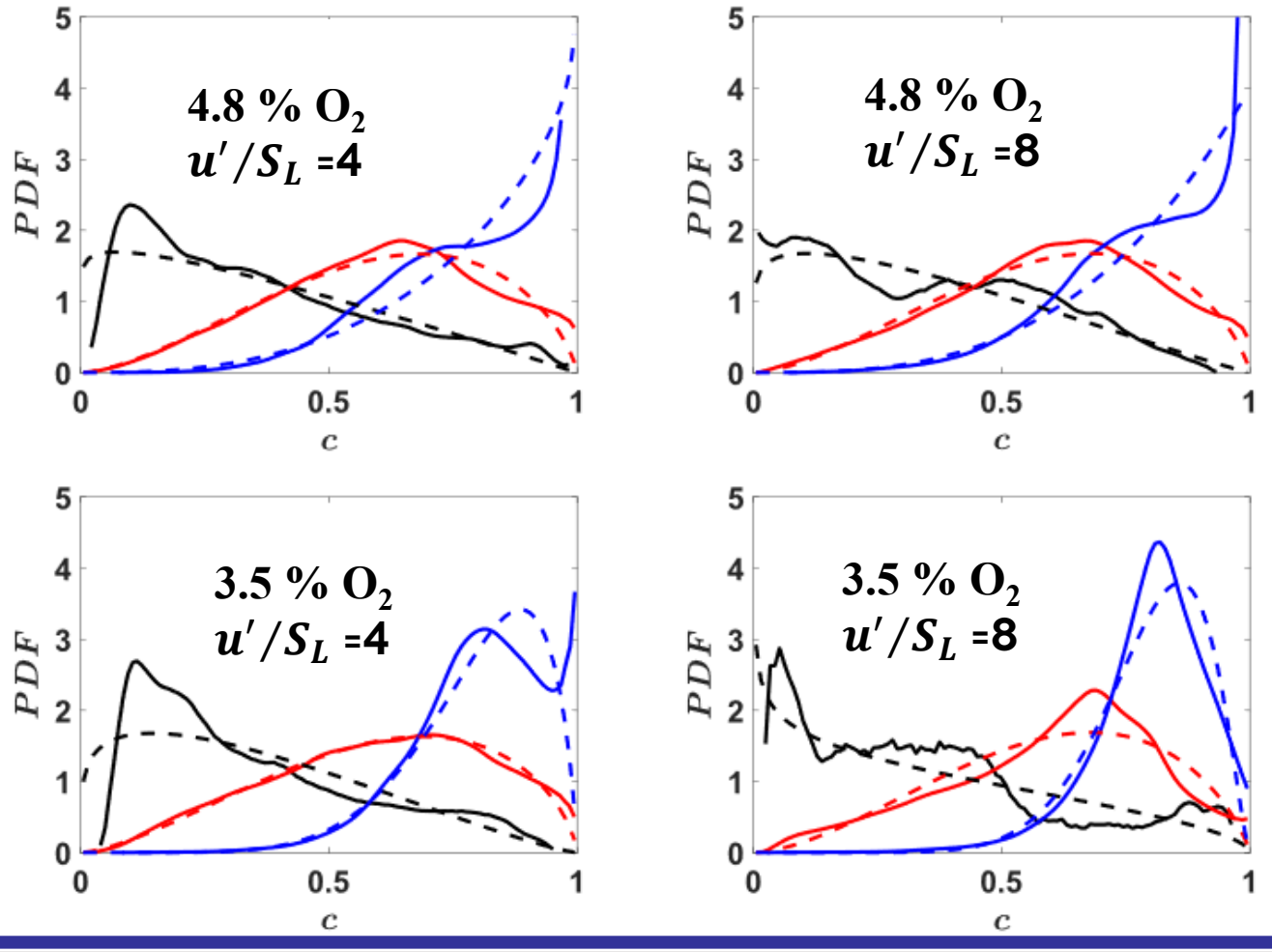
- Presuming the PDF requires the knowledge of first and second moments of the scalar in question.

- The beta-function is often used in the presumed PDF approach due to its flexibility, and it requires the knowledge of the reaction progress variable mean $\tilde{c}$ and variance $\widetilde{c''^2}$.

$$P(c) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} c^{a-1}(1-c)^{b-1} \quad \text{where } a = \tilde{c}\left[\frac{\tilde{c}\,(1-\tilde{c})}{\widetilde{c''^2}} - 1\right] \;;\; b = \frac{a}{\tilde{c}} - a$$

Presumed PDF approach (β-PDF)

- The β-PDF is a good representation for the progress variable in MILD combustion.



DNS: solid line
β-PDF: broken line

$\tilde{c} = 0.35$
$\tilde{c} = 0.60$
$\tilde{c} = 0.80$

Scalar dissipation rate (SDR) closure

- One of the most important unclosed terms in the $\widetilde{c''^2}$ transport equation is the scalar dissipation rate (SDR) and it closure is needed for the modelling of the $\widetilde{c''^2}$ transport equation

$$\frac{\partial(\overline{\rho}\widetilde{c''^2})}{\partial t}+\frac{\partial(\overline{\rho}\tilde{u}_j\widetilde{c''^2})}{\partial x_j}=-\frac{\partial}{\partial x_j}\left[\overline{\rho u_j''c''^2}\right]-2\overline{\rho u_j''c''}\frac{\partial\tilde{c}}{\partial x_j}+2\left[\overline{\dot{\omega}_c c}-\overline{\dot{\omega}_c}\tilde{c}\right]+\frac{\partial}{\partial x_j}\left(\bar{\rho}\widetilde{D}\frac{\partial\widetilde{c''^2}}{\partial x_j}\right)-2\overline{\rho}\widetilde{\epsilon_c}$$

- The Favre averaged scalar dissipation rate (SDR) is defined as [1]:

$$\widetilde{N_c}=\overline{\rho D\,\nabla c\cdot\nabla c}/\bar{\rho}=\widetilde{\varepsilon_c}+\widetilde{D}\,\nabla\tilde{c}\,.\nabla\tilde{c}$$

$$\text{where } \widetilde{\varepsilon_c}=\overline{\rho D\,\nabla c''\cdot\nabla c''}/\bar{\rho}$$

[1] Kolla, H., Rogerson, J.W., Chakraborty, N., Swaminathan, N.: Scalar dissipation rate modelling and its validation. Combust. Sci. Technol. 181, 518–535 (2009)

Scalar dissipation rate (SDR) closure

- Kolla et al. [1] proposed SDR closures for high Damköhler number (Da>>1) premixed flames.

$$\widetilde{N_C} = \left(2K_c^* \frac{S_L}{\delta_{th}} + C_3 \frac{\tilde{\varepsilon}}{\tilde{k}} - \boldsymbol{\tau}.C_4 \frac{S_L}{\delta_{th}}\right) \frac{\tilde{c}\,(1-\tilde{c})}{\beta_\varepsilon} + \tilde{D}\,\nabla\tilde{c}\,.\nabla\tilde{c} \quad (1)$$

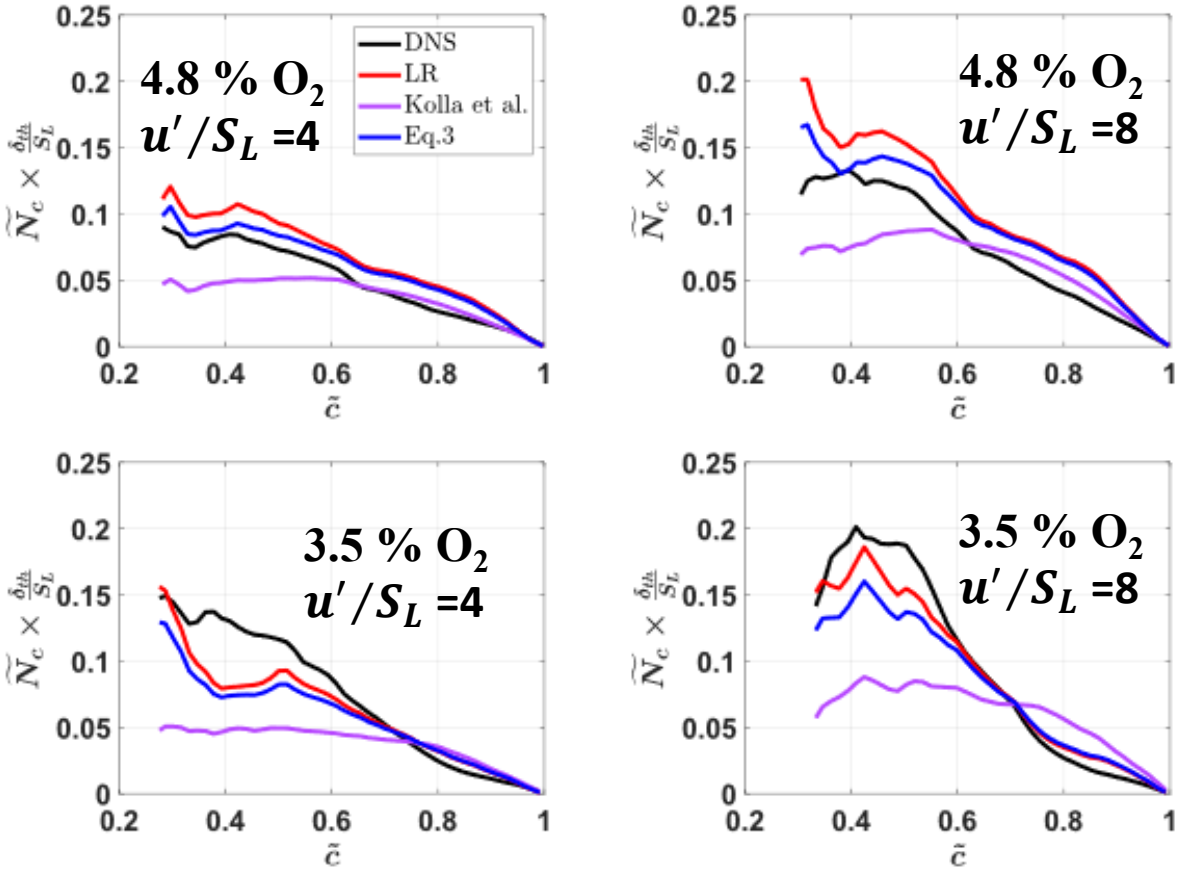
- SDR closure for passive scalar mixing (linear relaxation model) [2].

$$\widetilde{N_C} = C_\Phi \widetilde{c''^2} \frac{\tilde{\varepsilon}}{\tilde{k}} + \tilde{D}\,\nabla\tilde{c}\,.\nabla\tilde{c} \quad (2)$$

- Proposed SDR closure:

$$\widetilde{N_C} = s * Eq.1 + (1-s) C_\Phi \widetilde{c''^2} \frac{\tilde{\varepsilon}}{\tilde{k}} + \tilde{D}\,\nabla\tilde{c}\,.\nabla\tilde{c} \quad (3)$$

$$Where, s = \frac{\widetilde{c''^2}}{\tilde{c}(1-\tilde{c})} \quad \& \quad \boldsymbol{C_\Phi = \frac{0.029}{\tilde{c}^{2.7}} + 1.5}$$



[1] Kolla, H., Rogerson, J.W., Chakraborty, N., Swaminathan, N.: Scalar dissipation rate modelling and its validation. Combust. Sci. Technol. 181, 518–535 (2009)
[2] Mura, A., Robin, V., Champion, M.: Modelling of scalar dissipation in partially premixed flames. Combust. Flame 149, 217–224 (2007)

Eddy Break-Up and Eddy Dissipation Concept for mean reaction rate

- The modified EBU model includes the effect of the chemical reaction through 1-step reaction mechanism
  $\overline{\dot{\omega}_F} = -A\,\bar{\rho}\,\widetilde{Y}_L\,\frac{\tilde{\varepsilon}}{\tilde{k}}$ where $\widetilde{Y}_L = \min(\widetilde{Y}_f, \widetilde{Y_{ox}}/s)$ is mean limiting reactants and A is a model constant.

- The EDC assumes that the reacting regions occur at the fine structures and these structures are assumed to be in the same order as the Kolmogorov scales:

$$\overline{\dot{\omega}_i} = -\frac{\bar{\rho}\,\boldsymbol{\gamma_\lambda^2}}{\boldsymbol{\tau^*}(1-\boldsymbol{\gamma_\lambda^3})}\left(\widetilde{Y}_i - Y_i^*\right); \quad \boldsymbol{\tau^*} = C_{\boldsymbol{\tau}}\left(\frac{\tilde{\nu}}{\tilde{\varepsilon}}\right)^{1/2}, \quad \boldsymbol{\gamma_\lambda} = C_{\boldsymbol{\gamma}}\left(\frac{\tilde{\nu}\tilde{\varepsilon}}{\tilde{k}^2}\right)^{1/4}$$

where $C_{\boldsymbol{\tau}} = 0.4083$ and $C_{\boldsymbol{\gamma}} = 2.1377$

where $\boldsymbol{\tau^*}$ is the fine structure time fraction and $\boldsymbol{\gamma_\lambda}$ is the fine structure length fraction

- Different RANS studies suggested $C_{\boldsymbol{\tau}}$ =0.4083 to 3.0 and $C_{\boldsymbol{\gamma}}$ = 2.1377 to 1.0

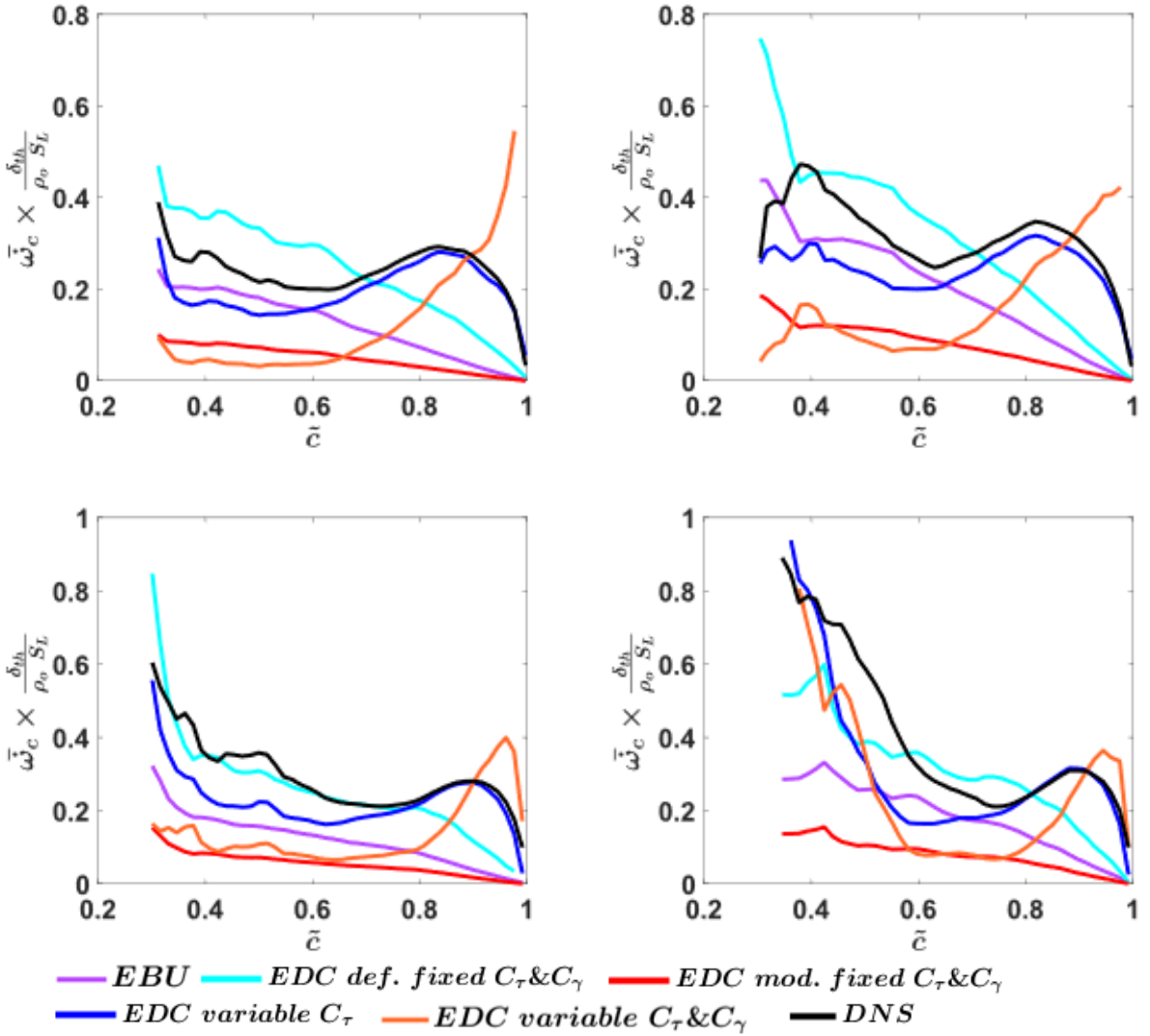
- Parente et al. [1] proposed functional relations for $C_{\boldsymbol{\tau}} \propto \frac{1}{Da_{\boldsymbol{\eta}}\sqrt{Re_T+1}}$ & $C_{\boldsymbol{\gamma}} \propto \sqrt{Da_{\boldsymbol{\eta}}(Re_T+1)}$

Where $Da_{\boldsymbol{\eta}} = \frac{t_f}{t_c}$ and $Re_T = \frac{\tilde{k}^2}{\tilde{\nu}\tilde{\varepsilon}}$

[1] Parente, A., Malik, M. R., Contino, F., Cuoci, A., & Dally, B. B. (2016). Fuel, 163, 98-111.

Eddy Break-Up (EBU) and Eddy Dissipation Concept (EDC)

- Overprediction for EBU and the EDC models with the fixed default model constants
- The EDC with the fixed modified model constants C_τ =3 and C_γ =1 underpredicts $\overline{\dot{\omega}_c}$
- The EDC with the variable model constant based on the expression by Parente et al. [1] underpredicts $\overline{\dot{\omega}_c}$ at low values of $\tilde{c}$
- The EDC with variable C_τ and fixed C_γ = 1.0 captures the behaviour of $\overline{\dot{\omega}_c}$



[1] Parente, A., Malik, M. R., Contino, F., Cuoci, A., & Dally, B. B. (2016). Fuel, 163, 98-111.

Flame surface density (FSD) and scalar dissipation rate (SDR) based mean reaction rate closure

- The closure of $\overline{\dot{\omega}_c}$ is utilised in the Flame Surface Density (FSD) model [1] through the expression:

$$\overline{(\rho S_d)_s}\,\Sigma_{\text{gen}} = \overline{\dot{\omega}_c} + \overline{\nabla.(\rho D \nabla c)}$$

in the context of RANS $\overline{\dot{\omega}_c} \gg \overline{\nabla.(\rho D \nabla c)}$ and $\overline{\nabla.(\rho D \nabla c)}$ is neglected.

Often $\overline{(\rho S_d)_s} \approx \rho_o S_L$ with the stretch factor $I_0 = 1.0$

$$\overline{\dot{\omega}_c} = \rho_o S_L\,\Sigma_{\text{gen}}$$

- The $\overline{\dot{\omega}_c}$ can be closed according to the following expression :

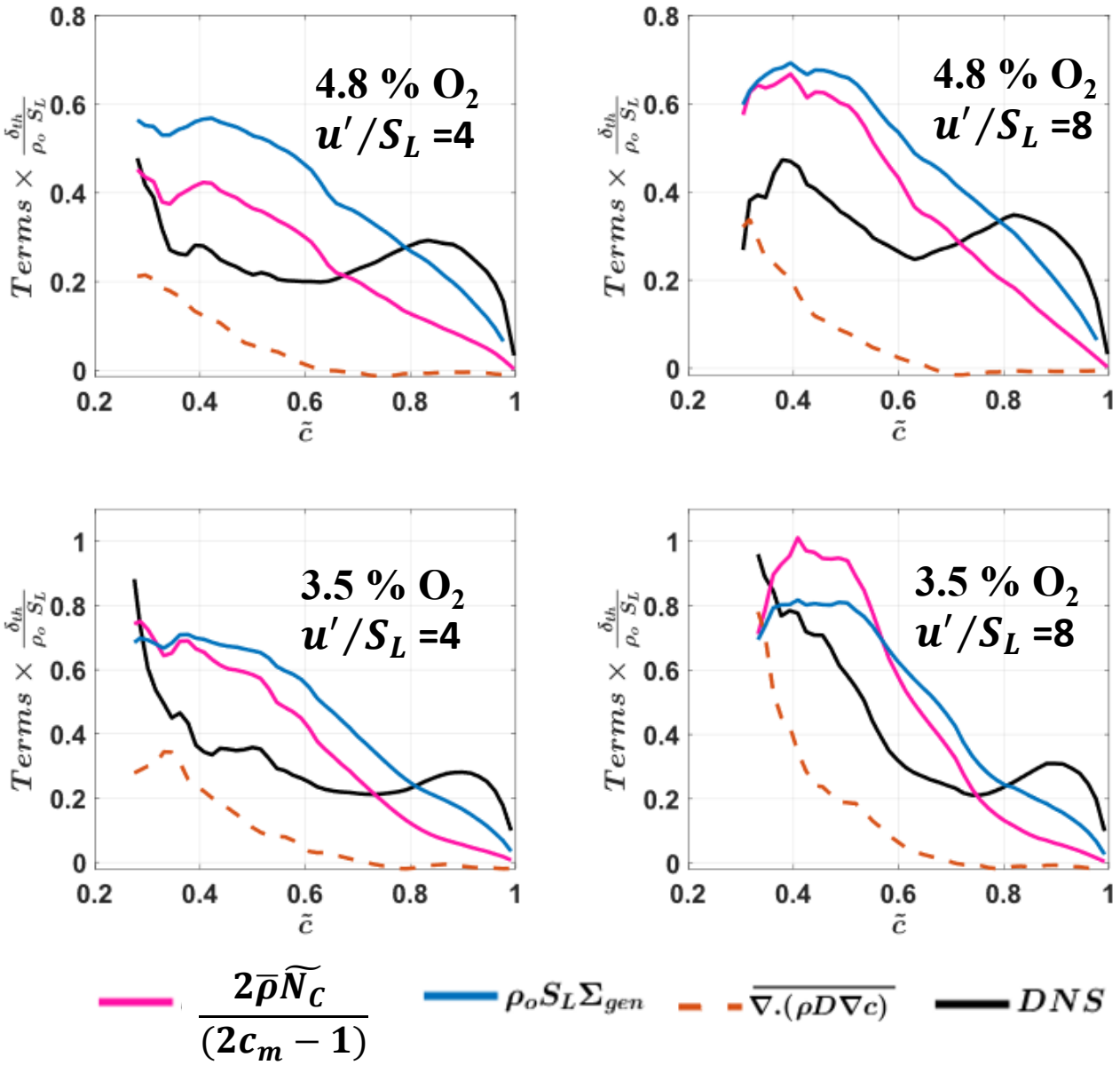
$$\overline{\dot{\omega}_c} = \frac{2\bar{\rho}\widetilde{N_C}}{(2c_m - 1)}$$

- The SDR closure is based on the infinitely fast chemistry assumption, however it is found to hold reasonably well in the thin reaction zone regime [2]

[1] A. Trouvé, T.J. Poinsot, J. Fluid Mech. 278, 1–131 (1994).
[2] N. Chakraborty, N. Swaminathan, Flow Turbulence Combust (2010), 10.1007/s10494-010-9305-.

FSD and SDR based mean reaction rate closure

- The SDR-based reaction rate closure overpredicts (underpredicts) the mean reaction rate at low (high) values of Favre average of progress variable $\tilde{c}$
- The molecular diffusion rate $\overline{\nabla \cdot (\rho D \nabla c)}$ assumes non-negligible values at low values of $\tilde{c}$ in MILD combustion
- Modelling $\overline{(\rho S_d)_s} \approx \rho_o S_L$ shows the same behaviour as the SDR-based mean ration rate closure



Conclusions

- The beta-function predicts the PDF of the reaction progress variable in MILD combustion
- It has been found that a linear relaxation closure for the SDR captures the behaviour of the SDR.
- The modified EBU and EDC with standard model coefficients overpredict the mean ration rate.
- When the EDC mixing time coefficient includes the effect of dilution using the functional expressions proposed by Parente et al.[1] , the EDC shows a good agreement with DNS.
- The SDR-based closures and the FSD approach with $\overline{(\rho S_d)}_s \approx \rho_o S_L$ overpredicts (underpredicts) the mean reaction rate at low (high) values of $\tilde{c}$

[1] Parente, A., Malik, M. R., Contino, F., Cuoci, A., & Dally, B. B. (2016). Fuel, 163, 98-111.

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Thank you