A priori DNS analysis of the closure of cross-scalar dissipation rate of reaction progress variable and mixture fraction in turbulent stratified flames

Peter Brearley Umair Ahmed Nilanjan Chakraborty

p.brearley@newcastle.ac.uk

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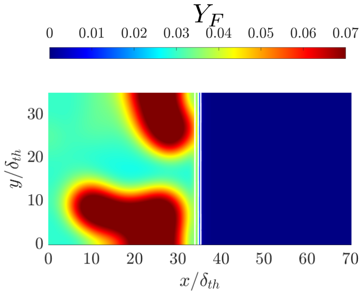
Turbulent Stratified Mixture Combustion

- It occurs when a limited mixing time is allowed between the unburned reactants such that some premixing takes place but not to the extent of homogeneity.
- It allows leaner overall mixtures to be used, reducing the burned gas temperature and NO_x emissions.
- A complete description of the flow requires a passive scalar (e.g. mixture fraction ξ) to describe the local mixture composition and an active scalar (e.g. reaction progress variable c) to determine the progress of the chemical reaction.



Cross-Scalar Dissipation Rate

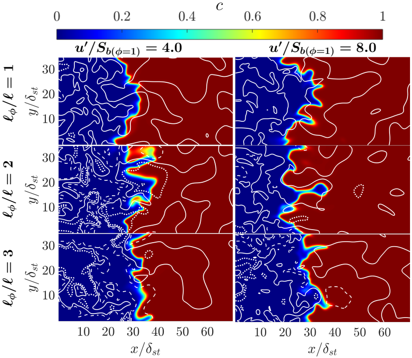
- Many modelling approaches require require solving the transport equations of the Favre averaged active and passive scalar variances $\widetilde{c''^2}$ and $\widetilde{\xi''^2}$, as well as their covariance $\widetilde{c''\xi''}$ to calculate the mean reaction rate. E.g.
  - Presumed probability density function[1]
  - Flamelet based tabulated chemistry[2]
  - Flamelet generated manifold[3]
- The cross scalar dissipation rate $\widetilde{\varepsilon_{c\xi}}$ is an important unclosed term appearing in the transport equation of $\widetilde{c''\xi''}$ and its closure is the focus of this study.
- Modelling of $\widetilde{\varepsilon_{Y_F\xi}}$ in the Libby-Williams framework has received lots of attention[4–6], but $\widetilde{\varepsilon_{c\xi}}$ has received very little attention.

[1] Libby & Williams (2000)
[2] Fiorina et al. (2015)
[3] Nguyen et al. (2010)
[4] Ribert et al. (2005)
[5] Robin et al. (2006)
[6] Malkeson & Chakraborty (2011)

Direct Numerical Simulation Database

- Six single-step chemistry with parameters $u'/S_{b(\phi=1)} = 4$ or 8, and initial $\ell_\phi/\ell = 1$, 2 or 3.[7]
- The activation temperature and heat of combustion are taken to be functions of equivalence ratio.[8]

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



[7] Brearley et al. (2020)
[8] Tarrazo et al. (2006)

Mathematical Definitions

- The cross-scalar dissipation rate is given by

$$\widetilde{\varepsilon_{c\xi}} = \frac{\overline{\rho D \nabla c'' \cdot \nabla \xi''}}{\bar{\rho}}, \qquad \widetilde{\varepsilon_{Y\xi}} = \frac{\overline{\rho D \nabla Y_F'' \cdot \nabla \xi''}}{\bar{\rho}}$$

where the mixture fraction ξ and reaction progress variable c are defined as

$$\xi = \frac{Y_F - Y_O/s + Y_{O\infty}/s}{Y_{F\infty} + Y_{O\infty}/s}, \qquad c = \frac{\xi Y_{F\infty} - Y_F}{\xi Y_{F\infty} - \max\left(0, \frac{\xi - \xi_{st}}{1 - \xi_{st}}\right) Y_{F\infty}}$$

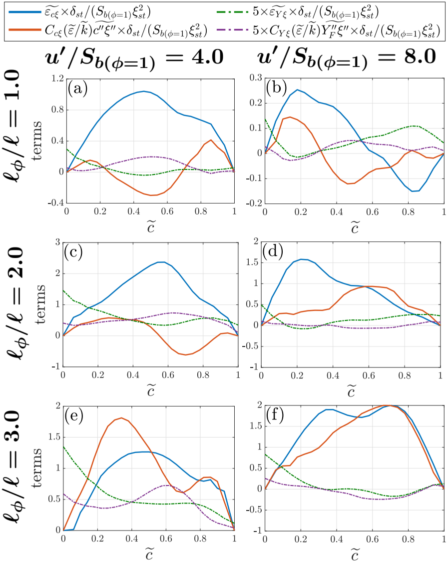
where $s = (Y_O/Y_F)_{st} = 4.0$ is the mass stoichiometric ratio for methane-air mixtures.

Algebraic Modelling

- The linear relaxation model

$$\widetilde{\varepsilon_{c\xi}} = C\frac{\widetilde{\varepsilon}}{\widetilde{k}}\widetilde{c''\xi''}, \quad \widetilde{\varepsilon_{Y\xi}} = C\frac{\widetilde{\varepsilon}}{\widetilde{k}}\widetilde{Y_F''\xi''}$$

- The linear relaxation model fails to accurately capture the $\widetilde{\varepsilon_{c\xi}}$ evolution throughout the flame.
- Since $\widetilde{\varepsilon_{c\xi}}$ can take on negative values, the $\sqrt{\widetilde{\varepsilon_c}}\sqrt{\widetilde{\varepsilon_\xi}}$ approximation is not valid.



Transport Equation Modelling

- The $\widetilde{\varepsilon_{c\xi}}$ transport equation is given by

$$\frac{\partial\left(\overline{\rho}\widetilde{\varepsilon_{c\xi}}\right)}{\partial t} + \frac{\partial\left(\overline{\rho}\widetilde{u}_j\widetilde{\varepsilon_{c\xi}}\right)}{\partial x_j} = \underbrace{\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial\widetilde{\varepsilon_{c\xi}}}{\partial x_j}\right)}_{D_1} \underbrace{+T_1 + T_2 + T_3 + T_4 - D_2}_{\text{unclosed terms}}$$

T_1 is the turbulent transport contribution

T_2 is the density variation contribution

T_3 is the scalar-turbulence interaction contribution

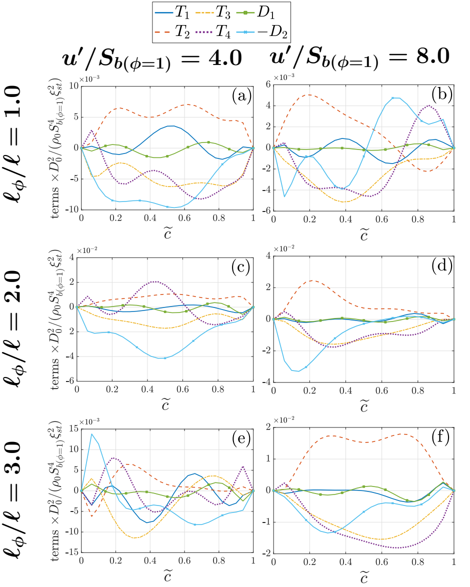
T_4 is the reaction rate contribution

D_1 is the molecular diffusion contribution

D_2 is the molecular dissipation contribution

Transport Equation Modelling: Statistical Behaviour

- T_1 plays a significant role for the small $u'/S_{b(\phi=1)}$ cases but diminishes as the turbulence intensity increases.
- D_1 plays an insignificant role in all cases, and can be neglected.
- The remaining terms (T_2, T_3, T_4, D_2) play leading order roles and have similar orders of magnitude.
- These observations have been reinforced by applying a scaling analyses.[9,10]



[9] Swaminathan & Bray (2005)
[10] Tennekes & Lumley (1972)

Transport Equation Modelling: T_1

Equation

$$T_{11} = -\frac{\partial}{\partial x_j} \overline{\left(\rho u_j'' \varepsilon_{c\xi} \right)}$$

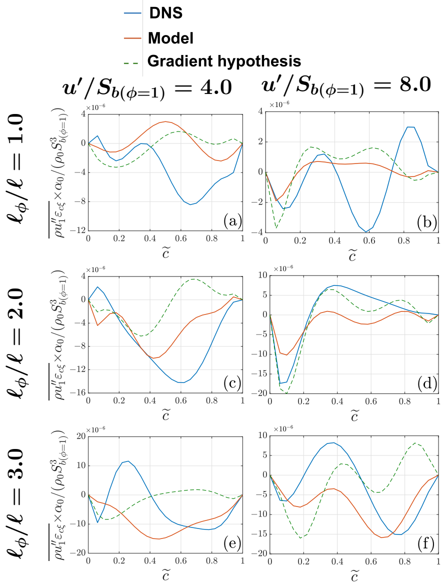
Model

$$\overline{\rho u_1'' \varepsilon_{c\xi}} = -\, g \frac{\mu_t}{\sigma_{c\xi}} \frac{\partial \widetilde{\varepsilon_{c\xi}}}{\partial x_1} - (1-g) \frac{\overline{\rho u_1'' c''}\ \overline{\rho u_1'' \xi''}}{\bar{\rho} \sqrt{\tilde{k}} \sqrt{\widetilde{c''^2}} \sqrt{\widetilde{\xi''^2}}}$$

$$g = \exp\left(-C \underbrace{\left[\left(\frac{\rho_0}{\bar{\rho}_b} - 1 \right) \frac{\overline{S_b}}{\sqrt{\tilde{k}}} \right]^2}_{\text{Bray number}} \right)$$

$$C = 0.5$$

- First term follows from the gradient hypothesis, and the second term is capable of predicting both gradient and counter gradient.



Transport Equation Modelling: T_2

Equation

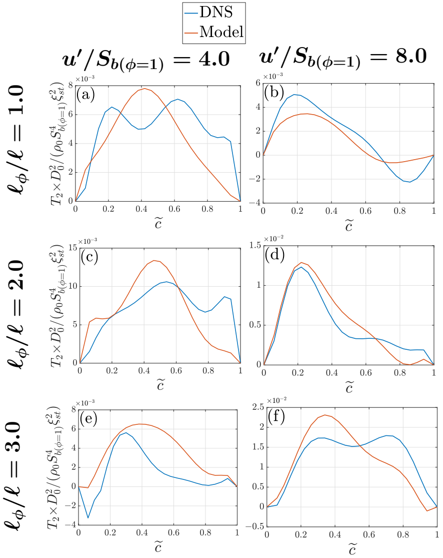
$$T_2 = \overline{-\frac{D}{\rho}\frac{\partial \rho}{\partial x_i}\left[\dot{\omega}_c\frac{\partial \xi}{\partial x_i} + \frac{\partial \xi}{\partial x_i}\frac{\partial}{\partial x_j}\left(\rho D \frac{\partial c}{\partial x_j}\right) + \frac{\partial c}{\partial x_i}\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial \xi}{\partial x_j}\right)\right]}$$
$$+ \frac{\bar{D}}{\bar{\rho}}\frac{\partial \bar{\rho}}{\partial x_i}\left[\overline{\dot{\omega}_c}\frac{\partial \tilde{\xi}}{\partial x_i} + \frac{\partial \tilde{\xi}}{\partial x_i}\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial \tilde{c}}{\partial x_j}\right) - \frac{\partial}{\partial x_j}\left(\overline{\rho u_j'' c''}\right)\frac{\partial \tilde{\xi}}{\partial x_i}\right.$$
$$\left. + \frac{\partial \tilde{c}}{\partial x_i}\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial \tilde{\xi}}{\partial x_j}\right) - \frac{\partial}{\partial x_j}\left(\overline{\rho u_j'' \xi''}\right)\frac{\partial \tilde{c}}{\partial x_i}\right]$$

Model

$$T_2 = K\bar{\rho}\widetilde{\varepsilon_{c\xi}}\widetilde{\varepsilon_c}\left(\frac{\rho_0}{\bar{\rho}_b} - 1\right)$$

$$K = 0.1 + \frac{0.15}{1+\exp\left(-0.5[Re_L - 15]\right)}$$

- Derived from scaling estimate of the expression, including appropriate density weighting.
- It is not sensitive to the degree of inhomogeneity, but is sensitive to turbulence intensity.



Transport Equation Modelling: T_3

- The scalar-turbulence interaction term is best modelled by grouping it into three subterms.

$$T_3 = T_{31} + T_{32} + T_{33}$$

$$\begin{aligned} T_{31} = & \left.-\overline{\rho D \frac{\partial c''}{\partial x_i}\frac{\partial u_j''}{\partial x_i}}\frac{\partial \widetilde{\xi}}{\partial x_j} - \overline{\rho D \frac{\partial c''}{\partial x_j}\frac{\partial u_j''}{\partial x_i}}\frac{\partial \widetilde{\xi}}{\partial x_i}\right\} T_{31}^{(i)} \\ & \left.-\overline{\rho D \frac{\partial \xi''}{\partial x_j}\frac{\partial u_j''}{\partial x_i}}\frac{\partial \widetilde{c}}{\partial x_i} - \overline{\rho D \frac{\partial \xi''}{\partial x_i}\frac{\partial u_j''}{\partial x_i}}\frac{\partial \widetilde{c}}{\partial x_j}\right\} T_{31}^{(ii)} \end{aligned}$$

$$T_{32} = -\overline{\rho D \frac{\partial c''}{\partial x_i}\frac{\partial \xi''}{\partial x_j}\frac{\partial u_j''}{\partial x_i}} - \overline{\rho D \frac{\partial c''}{\partial x_j}\frac{\partial \xi''}{\partial x_i}\frac{\partial u_j''}{\partial x_i}}$$

$$T_{33} = -\overline{\rho D \frac{\partial c''}{\partial x_j}\frac{\partial \xi''}{\partial x_i}}\frac{\partial \widetilde{u_j}}{\partial x_i} - \overline{\rho D \frac{\partial c''}{\partial x_i}\frac{\partial \xi''}{\partial x_j}}\frac{\partial \widetilde{u_j}}{\partial x_i}$$

Transport Equation Modelling: T_{31}

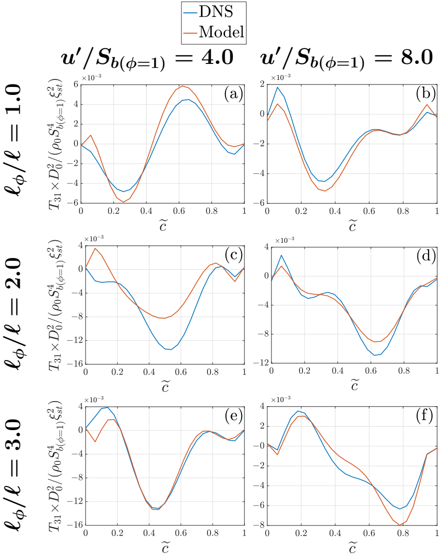
Equation

$$T_{31} = -\overline{\rho D \frac{\partial c''}{\partial x_i}\frac{\partial u_j''}{\partial x_i}}\frac{\partial \widetilde{\xi}}{\partial x_j} - \overline{\rho D \frac{\partial c''}{\partial x_j}\frac{\partial u_j''}{\partial x_i}}\frac{\partial \widetilde{\xi}}{\partial x_i}\Bigg\} T_{31}^{(i)}$$
$$- \overline{\rho D \frac{\partial \xi''}{\partial x_j}\frac{\partial u_j''}{\partial x_i}}\frac{\partial \widetilde{c}}{\partial x_i} - \overline{\rho D \frac{\partial \xi''}{\partial x_i}\frac{\partial u_j''}{\partial x_i}}\frac{\partial \widetilde{c}}{\partial x_j}\Bigg\} T_{31}^{(ii)}$$

Model

$$T_{31} = -C_1 \overline{\rho u_j'' c''}\frac{\widetilde{\varepsilon}}{\widetilde{k}}\frac{\partial \widetilde{\xi}}{\partial x_j} - C_2 \overline{\rho u_j'' \xi''}\frac{\widetilde{\varepsilon}}{\widetilde{k}}\frac{\partial \widetilde{c}}{\partial x_j},\ C_1 = 1, C_2 = 0.15$$

- $\overline{\rho D(\partial \xi''/\partial x_i)(\partial u_i''/\partial x_j)}$ and $\overline{\rho D(\partial c''/\partial x_i)(\partial u_i''/\partial x_j)}$ can be taken to scale with $\overline{\rho u_j'' \xi''}(\widetilde{\varepsilon}/\widetilde{k})$ and $\overline{\rho u_j'' c''}(\widetilde{\varepsilon}/\widetilde{k})$ based on previous modelling strategies.[11,12]



[11] Mantel & Borghi (1994)
[12] Chakraborty et al. (2008)

Transport Equation Modelling: T_{32}

Equation

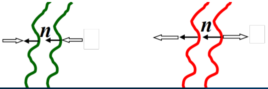
$$T_{32} = -\overline{\rho D \frac{\partial c''}{\partial x_i} \frac{\partial \xi''}{\partial x_j} \frac{\partial u_j''}{\partial x_i}} - \overline{\rho D \frac{\partial c''}{\partial x_j} \frac{\partial \xi''}{\partial x_i} \frac{\partial u_j''}{\partial x_i}}$$

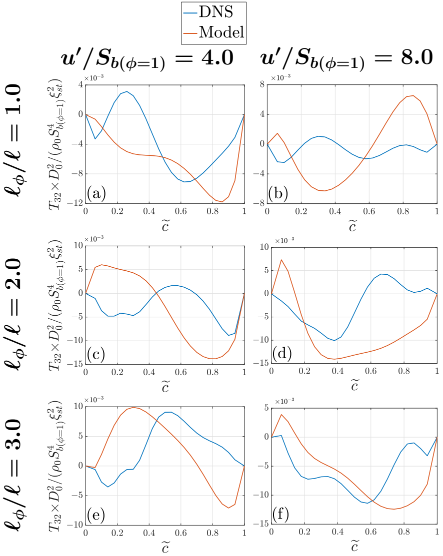
Model

$$T_{32} = \bar{\rho} \frac{\tilde{\varepsilon}}{\tilde{k}} \frac{\widetilde{\varepsilon_{c\xi}}}{\sqrt{|\widetilde{\varepsilon_{c\xi}}|}} \sqrt{\widetilde{\varepsilon_c}} \left[C_1 - C_2 \left(\frac{\rho_0}{\bar{\rho}_b} - 1 \right) Da_L \right]$$

$$C_1 = 0.028, C_2 = 0.01/(1 + Ka_L)^{0.5}$$

- The values and signs of T_{32} are determined by the relative competition of the strain rates due to turbulence and flame normal acceleration.





Transport Equation Modelling: T_{33}

Equation

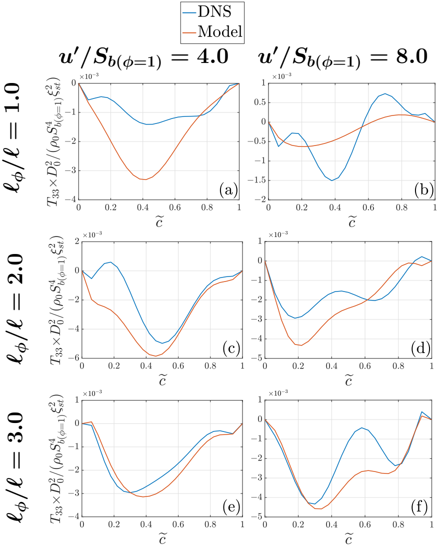
$$T_{33} = -\rho D \overline{\frac{\partial c''}{\partial x_j}\frac{\partial \xi''}{\partial x_i}\frac{\partial \widetilde{u_j}}{\partial x_i}} - \rho D \overline{\frac{\partial c''}{\partial x_i}\frac{\partial \xi''}{\partial x_j}\frac{\partial \widetilde{u_j}}{\partial x_i}}$$

Model

$$T_{33} = -C\bar{\rho}\widetilde{\varepsilon_{c\xi}}\frac{\partial \widetilde{u_1}}{\partial x_1}$$

$$C = 0.03$$

- The behaviour of T_{33} is expected to be affected by $\bar{\rho}\widetilde{\varepsilon_{c\xi}} \sim \overline{\rho D(\partial c''/\partial x_1)(\partial \xi''/\partial x_1)}$ and $\partial\widetilde{u_1}/\partial x_1$.



Transport Equation Modelling: $T_4 - D_2$

Equation

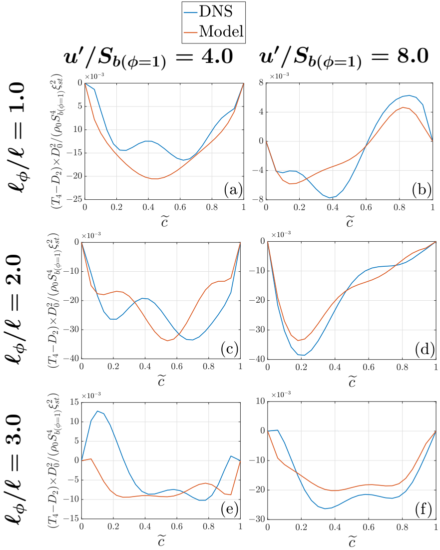
$$T_4 - D_2 = \overline{D\frac{\partial \dot{\omega}_c}{\partial x_i}\frac{\partial \xi}{\partial x_i}} - \overline{D}\frac{\partial \overline{\dot{\omega}_c}}{\partial x_i}\frac{\partial \widetilde{\xi}}{\partial x_i}$$
$$- \left(\overline{2\rho D^2 \frac{\partial^2 c}{\partial x_i \partial x_j}\frac{\partial^2 \xi}{\partial x_i \partial x_j}} - 2\overline{\rho}\,\overline{D}^2 \frac{\partial^2 \widetilde{c}}{\partial x_i \partial x_j}\frac{\partial^2 \widetilde{\xi}}{\partial x_i \partial x_j}\right)$$

Model

$$T_4 - D_2 = \bar{\rho}\frac{\widetilde{\varepsilon_{c\xi}}\widetilde{\varepsilon_{\xi}}}{\widetilde{\xi''^2}}\left[1 + \left(\frac{c}{1+c}\right)^2\right]\left[C_1(0.2m - \widetilde{c}) - C_2 m\right]$$

$$C_1 = 0.35, C_2 = 0.4, m = \frac{\overline{S_b}\sqrt{\widetilde{\xi''^2}}/D_0\widetilde{\varepsilon}_\xi}{1 + \overline{S_b}\sqrt{\widetilde{c''^2}}/D_0\widetilde{\varepsilon}_\xi}$$

- T_4 and D_2 can be very large terms and their difference is important, so they are commonly modelled together. However, the models also perform well individually.



Conclusions

- The density variation term T_2, scalar-turbulence interaction term T_3, the reaction rate contribution T_4 and the molecular dissipation term $-D_2$ are the leading order contributors.
- T_1 is small in comparison to the leading order contributors.
- The new models predict the unclosed terms of the $\widetilde{\varepsilon_{c\xi}}$ transport equation satisfactorily for all the cases, but this is one of the first attempts to model this, so there is scope for improvement for some of the terms.
- Future research should address the effects of detailed chemistry and differential diffusion for higher turbulent Reynolds numbers.
- The models proposed require RANS implementation where experimental data is available for the purpose of *a posteriori* assessment of the models.

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