Turbulence-chemistry interaction modelling with extended Eddy Dissipation Concept and Partially Stirred Reactor in MILD combustion regime

M.T. Lewandowski[1], Z. Li[2], A. Parente[2], J. Pozorski[1]

[1.] *Institute of Fluid Flow Machinery, Polish Academy of Sciences, Gdańsk, Poland*
[2.] *Aero-Thermo-Mechanics Laboratory, Université Libre de Bruxelles, Brussels, Belgium*

Introduction

Moderate and/or Intense Low Oxygen Dilution (MILD) combustion is one of promising clean combustion technologies with high efficiency, low pollutant emissions and suitable for various fuels [1]. However, the physics of this regime is not fully understood and obtaining MILD conditions in industrial devices is still a hot topic. Numerical simulations are nowadays an essential tool assisting in the design process. The characteristic features of MILD regime differ from standard combustion and the numerical modelling of turbulence-chemistry interaction appears to be a challenging task. Therefore, it is essential to develop a robust, accurate numerical model feasible for industrial applications, accounting for the finite rate, detailed chemistry. Recent DNS studies [2] have revealed that reactor type models suitable for modeling MILD conditions. In this work we analyse and compare two popular reactor type models and their recent extensions to MILD regime [3, 4]. Those modifications aim to extend the models' applicability by adjusting to the local conditions, contrary to the usually proposed *ad hoc* tuning of the global constants, preserving generality of such approach.

Methodology

There is a wide choice of turbulence–chemistry interaction models for the standard turbulent premixed or non-premixed combustion. In MILD conditions, where the reaction zone is considerably different than in standard combustion, the smallest turbulence scales strongly affect the reaction zones and laminar flame structures are difficult to identify [2]. Advanced and accurate transported PDF or Conditional Moment Closure methods are still computationally unaffordable for industrial applications. Therefore simplified methods are extremely needed and among them the Flamelet Generated Manifold [5, 6] approach and mixing reactor models [7, 8, 9] have been extensively developed in recent years. In the former approach finding an appropriate parameterisation of the reaction zone becomes a challenge, whereas in the latter one, various formulations exist (PDF-PSR, PaSR, EDC) that need to be extended for MILD conditions. In this work we have focused on the Eddy Dissipation Concept (EDC) [10] and Partially Stirred Reactor (PaSR) [11] using Reynolds Averaged Navier-Stokes approach within open source software OpenFOAM.

The EDC is based on the turbulence energy cascade model [12] where the mean reaction rate for specie i is expressed as

$$\bar{R}_i = \frac{\bar{\rho}\gamma_\lambda^2\chi}{\tau^*(1-\gamma_\lambda^2\chi)}\left(Y_i^* - \tilde{Y}_i\right), \qquad (1)$$

where $\bar{\rho}$ is density, γ_λ and τ^* are the EDC parameters describing the small scale turbulence structures where reactions take place and they are functions of the mean flow turbulence quantities k and ε. Those structures are characterised by the reacting fraction χ usually set to unity. Quantity Y_i with tilde is the mean mass fraction of specie i, whereas Y_i^* is the respective mass fraction in the fine structures, which need to be obtained as a solution of ordinary differential equations representing the perfectly stirred reactor (PSR). In the extension of

corresponding author: Michał T. Lewandowski email: milewandowski@imp.gda.pl

Parente et al. [7], the definitions of γ_λ and τ^* additionally took into account the effects of slow chemistry and low turbulence (characteristic of MILD conditions) by the relations

$$\tau^* = \underbrace{\frac{1}{2}\frac{1}{Da_\tau\sqrt{C_\mu Re_\tau+1}}}_{C_\tau}\sqrt{\frac{\nu}{\varepsilon}}, \quad \text{and} \quad \gamma_\lambda = \underbrace{\sqrt{\frac{3}{2}}\sqrt{Da_\tau(C_\mu Re_\tau+1)}}_{C_\gamma} Re_\tau^{-1/4}, \tag{2}$$

where Da_τ is a local Damköhler number evaluated at the Kolmogorov scale and $Re_\tau = k^2/\nu\varepsilon$ is the turbulence Reynolds number. In standard EDC, C_τ and C_γ are constant values equal to 0.408 and 2.13, respectively. Here, they are variable parameters bounded between their standard value and 5.0 and 0.5, respectively. In the work of Lewandowski and Ertesvåg [8], the concept of variable χ originally proposed in [10], was reconsidered and adopted to MILD combustion regime. In this work both concepts are applied formulating the hybrid model [4] schematically presented in Fig. 1 (right).

The PaSR model is closely related to the EDC, yet instead of using cascade model it assumes that the computational cell is split into reacting and non-reacting locally uniform zones. The mass fraction of the reacting zone is estimated as [11]

$$\kappa = \frac{\tau_{ch}}{\tau_{ch}+\tau_m}, \tag{3}$$

where τ_{ch} and τ_m are the characteristic chemical and mixing time scales, respectively. The challenge here is to properly estimate those scales with an appropriate approach. As mentioned earlier in MILD regime characteristic scales differ from those in traditional combustion, thus standard approaches must be revised and relevant ones selected [3]. In conventional combustion it is accurate to assume that the mixing scale is of the order of the Kolmogorov one $\tau_K = \sqrt{\nu/\varepsilon}$. Ferrarotti et al. [9] showed that for MILD combustion it is more accurate to use the dynamic estimation of the mixing time scale based on the ratio of the scalar variance to the scalar dissipation rate $\tau_m = \widetilde{\phi''^2}/\widetilde{\varepsilon_\phi}$. Using mixture fraction f as a scalar describing the mixing process one has to solve additional transport equations for the mean mixture fraction $\tilde{f}$, mixture fraction variance $\widetilde{f''^2}$ and mixture fraction dissipation rate $\tilde{\chi}$. Chemical time scale was estimated from formation rates. It is worth to point out that calculations in both EDC and PaSR can be accelerated with the use of chemistry reduction and tabulation algorithms [13].

To assure a wide range of applicability of the analysed models, validation was based on Jet-in-Hot-Coflow (JHC) burner configuration which enables experimental investigations of MILD conditions in a laboratory scale. Data from two JHC burners from Delft [14] and Adelaide [15] were acquired for the purpose of the present work and twelve flames (see Fig. 1 and Table 1) were simulated using variants of EDC and PaSR. Turbulence boundary conditions were taken from the experimental data and estimated with the expressions proposed in [16].

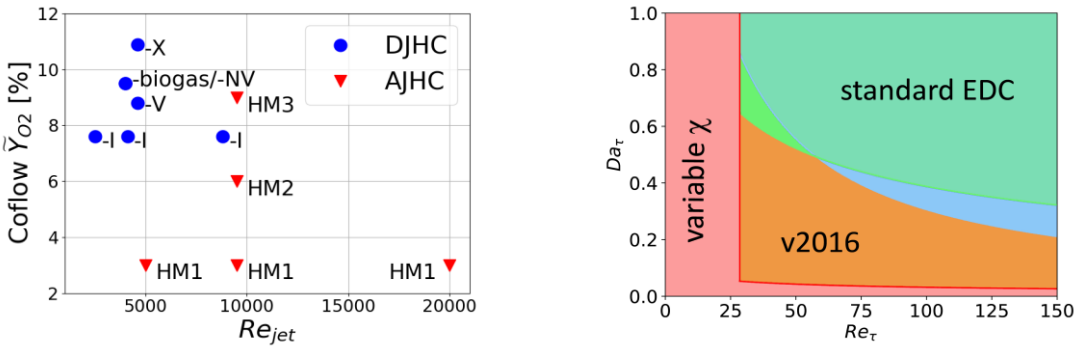

Figure 1. *Characterisation of the Adelaide and Delft JHC flames: plot of jet Reynolds number vs the level of oxygen content in the coflow (left). Hybrid EDC model presented in Re_τ vs Da_τ diagram (right), where v2016 denotes model from [7] and variable χ denotes model from [8].*

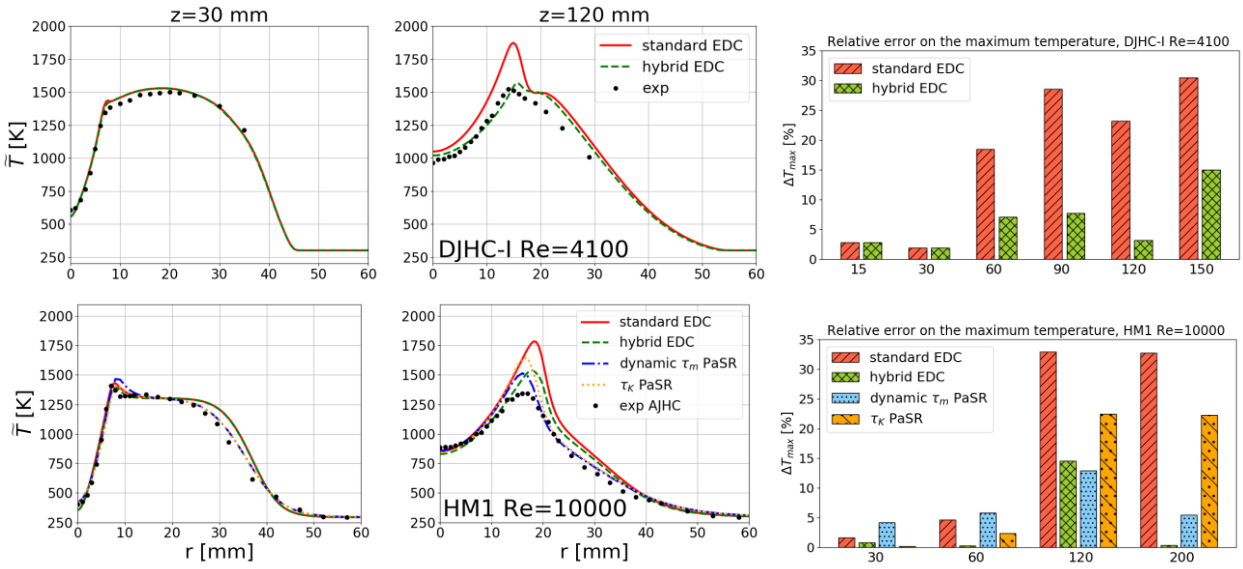

Figure 2. *First two columns show radial temperature distribution for the Delft and Adelaide JHC flames (first and second row, respectively) at the distances 30 mm and 120 mm. The third column presents relative error of the temperature peak in each axial location. Two variants of EDC were used for DJHC flames and for AJHC cases additionally two variants of PaSR were applied.*

Results

A number of simulations have been performed to have an opportunity for a broad comparative study between the selected approaches. Prior to the assessment of combustion models, a detailed sensitivity analysis of the boundary conditions, chemical mechanism, turbulence models, radiation, multicomponent diffusion and other aspects of physical modelling was performed. In Fig. 2 the temperature results for the Delft JHC flame at *Re*=4100 and Adelaide JHC at *Re*=10000 are shown. At the moment, for the Delft flame only the EDC results are compared showing a considerable improvement in predicting the maximum temperature value with the hybrid EDC. For the AJHC case both standard and extended PaSR and EDC are compared. It is clear that the standard EDC provided the highest error in the maximum temperatures downstream the flame. At the same time both model modifications provided improved results with very similar maximum temperature value at 120 mm. In many studies of the AJHC flames it has been shown that at the location 120 mm the model predictions are prone to errors. Thus Fig. 3 shows temperature and OH mass fractions at that location for the three flames with different levels of oxygen in the coflow (3%, 6% and 9%). The PaSR model with dynamic mixing time scale provided comparable temperature distributions to the ones obtained with the hybrid EDC and both agree well with the experiment. More pronounced differences can be observed in the predictions of hydroxyl radical, where for the HM1 flame the PaSR results perfectly corresponded to the experimental data and the hybrid EDC overestimated the peak value. On the other hand, for the cases HM2 and HM3 the PaSR model led to the OH underestimation, whereas hybrid EDC overestimated the peak value but not as much as in HM1 case. Also the effect of fuel type was captured with both models correctly.

Table 1. *The characteristic parameters of the flames.*

	Reynolds number	Coflow oxygen content	Fuel composition (by volume)
DJHC	2500, 4100, 8800	7.6%, 8.8%, 10.9%	15 % N_2 , 81 % CH_4, 4 % C_2H_6
	4000	9.5%	10.5 % N_2 , 56.7 % CH_4, 2.87 % C_2H_6, 30% CO_2
AJHC	5000, 10000, 20000	3% , 6%, 9%	50 % H_2 , 50 % CH_4

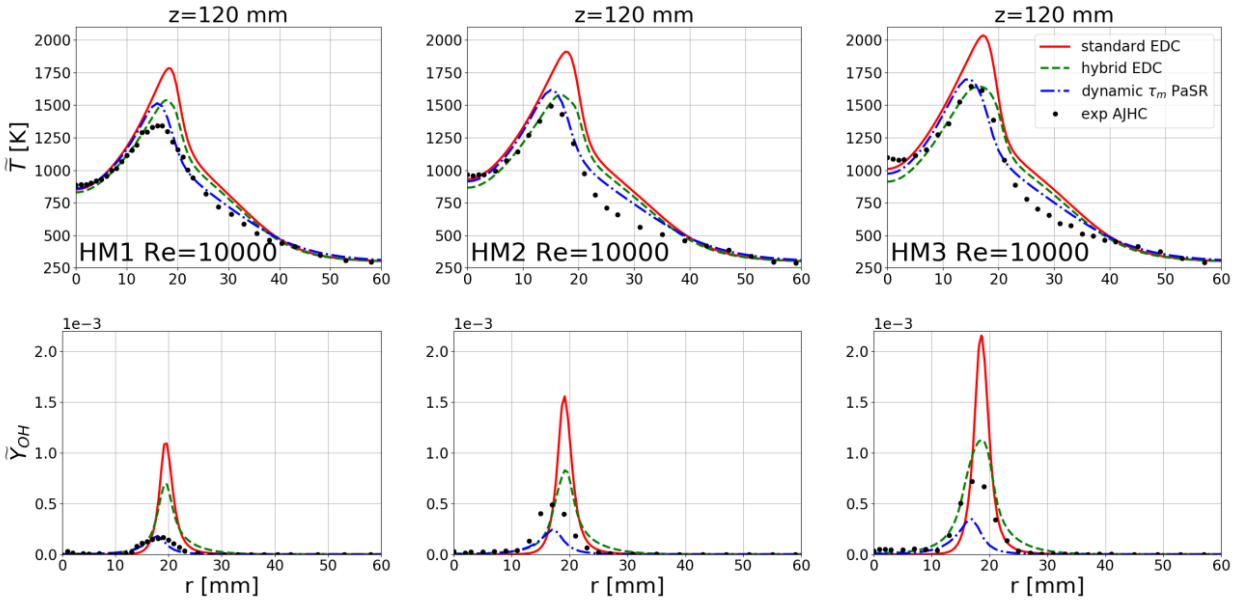

Figure 3. *The temperature (first row) and OH mass fraction (second row) radial distributions at the axial position 120 mm downstream of the nozzle for the three Adelaide JHC flames denoted as HM1, HM2 and HM3, with oxygen content in the coflow stream of 3%, 6% and 9% respectively.*

Conclusions

Based on the large number of laboratory burner simulations prepared with great care, we have shown that the modifications proposed by the authors considerably improved the species concentrations, the lift-off predictions and successfully alleviated the commonly reported problem of temperature overestimation by the standard EDC. Temperature and major species predictions obtained with PaSR using dynamically estimated mixing time scale were comparable to the hybrid EDC results. More pronounced differences appeared in case of minor species such as OH. At this stage PaSR simulations were performed only for the AJHC flames. Having in mind different local flow conditions in both JHC burners it is essential to validate PaSR model in DJHC flames fuelled with natural gas and biogas. The use of RANS methodology implies the problem of non-generality. Therefore, attention has to be paid to a careful model analysis, adjustment, calibration and validation on a wide range of operating conditions and various fuel mixtures.

References

[1] Cavaliere A., de Joannon M., *Prog. Energ. Combust. Sci.* **30** (2004) 329–366;
[2] Minamoto Y., Swaminathan N., Cant S., Leung T., *Combust. Flame* **161** (2014) 2801–2814;
[3] Li Z., Ferrarotti M., Cuoci A., Parente A., *Applied Energy* **225** (2018) 637–655;
[4] Lewandowski M.T, PhD Thesis, Gdańsk, Poland 2018;
[5] Göktolga M.U., van Oijen J.A., de Goey L.P.H., *Proc. Combust. Inst.* **36** (2017) 4269–4277;
[6] Sorrentino G., Ceriello G., de Joannon M., Sabia P., et al., *Energy and Fuels* **32** (2018) 10242–10255;
[7] Parente A., Malik M.R., Cantino F., Cuoci A., and Dally B.B., *Fuel* **163** (2016) 98–111;
[8] Lewandowski M.T., Ertesvåg I.S., *Fuel* **224** (2018) 687–700;
[9] Ferrarotti M., Li Z., Parente A., *Proc. Combust. Inst.* (2018) (in press);
[10] Gran I.R., Magnussen B.F., *Combust. Sci. Tech.* **119** (1996) 171-190, 191–217;
[11] Chomiak J., Karlsson A., *Symposium (Int.) on Combustion* **26** (1996) 2557–2564;
[12] Ertesvåg I.S., Magnussen B.F., *Combust. Sci. Technol.* **159 (**2000) 213–235;
[13] Li Z., Lewandowski M.T., Contino F., Parente A., *Energy and Fuels* **32** (2018) 10121–10131;
[14] Oldenhof E., Tummers M., van Veen E., Roekaerts D., *Combust. Flame* **158** (2011) 1553–1563;
[15] Dally B.B., Karpetis A.N., Barlow R.S., *Proc. Combust. Inst.* **29** (2002) 1147–1154;
[16] Lewandowski M.T., Płuszka P., Pozorski J., *Int. J. Num. Meth. Heat Fluid Flow* **28** (2018) 1433–56.