



ELSEVIER

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Full Length Article

Generalised Eddy Dissipation Concept for MILD combustion regime at low local Reynolds and Damköhler numbers. Part 2: Validation of the model

 Michał T. Lewandowski^{a,b,*}, Zhiyi Li^c, Alessandro Parente^{c,d}, Jacek Pozorski^a
^a Institute of Fluid Flow Machinery, Polish Academy of Sciences, Gdańsk, Poland

^b Department of Energy and Process Engineering, NTNU Norwegian University of Science and Technology, Trondheim, Norway

^c Aero-Thermo Mechanics Laboratory, Université Libre de Bruxelles, Brussels, Belgium

^d Combustion and Robust Optimization Group (BURN), Université Libre de Bruxelles and Vrije Universiteit Brussel, Brussels, Belgium

ARTICLE INFO

Keywords:

MILD combustion

Modelling

Eddy Dissipation Concept

Jet-in-Hot-Coflow

Reynolds and Damköhler numbers

turbulence inlet boundary conditions

ABSTRACT

The generalised Eddy Dissipation Concept (EDC) developed in the first part of this article is thoroughly validated against twelve flames from the Delft and Adelaide jet-in-hot-coflow (JHC) burners. These flames emulate Moderate or Intense Low Oxygen Dilution (MILD) conditions. Modelling of turbulence-chemistry interactions in this regime is a non trivial problem and many standard combustion models may fail. Recent Direct Numerical Simulation studies revealed a distributed appearance of the reaction zone indicating non-flamelet regime, which justified the use of reactor type modelling approaches. Those kind of models are of empirical nature and are sometimes criticized for being dependent on a number of tunable parameters. Also, most of new concepts are validated against a limited number of experiments. In this study, using the same modelling setup, twelve flames with different jet Reynolds number, level of oxidizer dilution with various fuel mixture were simulated. It turned out that the generalised EDC model considerably improved predictions with respect to the standard model for all the considered flames. Even though the predictions of the other EDC extensions provided better results in some regions, only the proposed generalised approach could cover the broad range of operating conditions, proving its “universality” and reliability.

1. Introduction

Moderate or Intense Low Oxygen Dilution (MILD) combustion is gaining increasing interest for the development of new technologies, as explained in the first part of this study [1]. In particular, this regime allows to couple very high energy efficiency with low pollutant emissions, for variety of fuels. A key requirement to operate in MILD combustion is a strong recirculation of exhaust gases into the fresh air, to preheat the charge and reduce the oxygen concentration. In the laboratory-scale flames, this can be achieved with Jet-in-Hot-Coflow (JHC) burners [2,3], where the recirculation is replaced by a co-flow issuing for a secondary burner. The advantage of this configuration is the availability of high fidelity data and the possibility of isolating the reaction in diluted conditions from the actual recirculation process. In addition, generation of vitiated gases in the coflow stream provides good control over the local composition [4]. Such an axisymmetric burner in non-enclosed environment enables conduction of optical measurements which provide insight into the unique features of MILD regime. The collected data can be used in the validation of various

numerical models. To ensure the generality of the proposed generalised EDC model a single case is obviously not enough. A complete assessment is carried out under several conditions and different fuels. Series of measurements with various jet Reynolds numbers, levels of coflow dilution and fuel types are analysed to test the models for wide range of operating conditions. This is especially important for the Reynolds Averaged Navier-Stokes (RANS)-based models, which may encounter problems at low and high turbulence.

The flames issuing from the JHC burners have been numerically investigated in many previous papers. Especially, extensive studies can be found on the Adelaide [5–19] and Delft [20–26] flames. Selected approaches have been discussed in the first part of this study [1]. Recently, Perpignan et al. [4] presented a complete review of modelling approaches applied to the JHC configuration. They pointed out that, due to the uncertainties related to the underlying physics of MILD combustion, most of the known turbulence-chemistry interaction (TCI) approaches have been already assessed in this regime. They considered different turbulence-chemistry interaction models based on presumed Probability Density Function (PDF), flamelets, transported PDF,

* Corresponding author at: Department of Energy and Process Engineering, NTNU Norwegian University of Science and Technology, Trondheim, Norway.

E-mail address: michalew@ntnu.no (M.T. Lewandowski).

<https://doi.org/10.1016/j.fuel.2020.117773>

Received 8 July 2019; Received in revised form 1 February 2020; Accepted 2 April 2020

Available online 25 June 2020

0016-2361/ © 2020 The Author(s). Published by Elsevier Ltd. This is an open access article under the CC BY license

(<http://creativecommons.org/licenses/by/4.0/>).

Flamelet Generated Manifold (FGM), Conditional Moment Closure (CMC) and the Eddy Dissipation Concept (EDC). The EDC was indicated as the most used closure for turbulence-chemistry interactions due to its availability in different computational codes, easiness of incorporating diverse reaction mechanisms and its long standing tradition in the field. The model was reported to provide reasonably accurate results if appropriately modified. According to Perpignan et al. [4], if a robust and flexible modification of the EDC model is developed, it can become even more popular. In the first part of this study [1], the limitations associated to the standard EDC were reported, potential improvements were discussed and its generalization introduced.

The EDC for turbulence-chemistry interaction was proposed by Gran and Magnussen [27], and recently extensively investigated for MILD combustion regime [5,7,6,15,20,25,28,29]. Based on our previous research [5,25], in the first part of this study [1] we have extended the range of applicability of the EDC model by ensuring proper behaviour under extremely low Reynolds and Damköhler numbers conditions. The present formulation is based on functional expressions where the model parameters are adjusted to the local conditions in terms of Reynolds and Damköhler numbers, contrary to the usually proposed *ad hoc* tuning of the global EDC constants.

2. Laboratory scale burners

The laboratory test cases selected for this study are non-premixed flames where the fuel jet is surrounded by a hot and diluted coflow. Auto-ignition occurs in the shear layer between the two streams. The advantage of this configuration is the availability of high fidelity data and the possibility of isolating the reaction in diluted conditions from the actual recirculation process. Two JHC burners from Adelaide (AJHC) [3] and Delft [2] (DJHC) were considered and data from twelve flames were acquired. As pointed out by De and Dongre [21] both experimental burners configurations are similar but jointly provide a complementary detailed database to study the JHC flames. A schematic design and the detailed description of the two burners is presented in [3,2]. Their characteristics such as the jet Reynolds number and the level of oxygen dilution together with flames notation are presented in Fig. 1.

Although the design of the two burners is very similar it has to be pointed out that, for the AJHC flames, scalar data measurements are available including temperature, major and selected minor species. In case of DJHC burner, velocity and Reynolds stresses measurements were taken, contrary to the AJHC. However, only temperature is available in terms of scalars. The Reynolds stresses allowed to directly calculate turbulence inlet conditions without need of performing additional cold flow simulations or adjustments as in case of Adelaide flames [7,12,13]. Delft flames operate at lower jet Reynolds number, and hence are very useful to investigate MILD combustion under at low

level of turbulence. Observing and comparing similar effects in both configurations (AJHC and DJHC) under different turbulence levels, oxidizer dilution and fuel composition provides a broad overview on the modelling needs in low local Damköhler and Reynolds numbers conditions. It should be also pointed out after Oldenhof et al. [30], that applying the conclusions drawn from the Jet-in-Hot-Coflow flames to industrial MILD combustion burners should be done with care. This circumspection comes from differences in JHC flames structure compared to industrial burners, where the strong turbulent motion plays an important role.

2.1. Adelaide JHC burner

The configuration of the Adelaide JHC (AJHC) burner consists of a central primary fuel jet with 4.25 mm inner diameter, surrounded by an annular coflow with a diameter of 82 mm. The central jet fuel pipe is insulated, cooled and provides an equimolar mixture of CH_4 and H_2 . The coflow stream is also generated by a secondary burner, which provides hot combustion products mixed with air and nitrogen to obtain the desired amount of oxygen level at the exit. The burner is mounted in a wind tunnel with cross section of 254 mm \times 254 mm. A series of experiments considered in this study consists of five flames, all fuelled with the same mixture but differing for the jet Reynolds number (Re) and the oxygen amount in the coflow. Flames denoted as HM1, HM2 and HM3 are all characterised by $Re = 10000$ and have 3%, 6% and 9% (by mass) oxygen in the coflow, respectively. The case HM1 was additionally investigated at three jet Reynolds numbers 5000, 10000 and 20000. For those flames, the measured species concentrations, mixture fraction and temperature are available at the centerline and four axial locations 30 mm, 60 mm, 120 mm and 200 mm. The scalars were measured instantaneously and simultaneously using the single-point Raman-Rayleigh laser induced fluorescence technique [3].

2.2. Delft JHC burner

The Jet-in-Hot-Coflow burner from Delft (DJHC) is similar to the one from Adelaide. In this configuration, the inner diameter of the central jet nozzle is equal to 4.5 mm and the coflow has the inner diameter of 82.8 mm. The coflow stream is generated by a partially premixed combustion of the same fuel. A series of experiments with different fuel mass flow rates and coflow conditions with different oxygen content, temperature and mass flow rate were carried out by Oldenhof et al. [2]. In the first modelling study of EDC analysis, the flame denoted as DJHC-I [20,2] was considered with three different fuel mass flow rates resulting in a jet Reynolds numbers of 2500, 4100 and 8800. The composition of the Dutch natural gas was specified as 15% N_2 , 81% CH_4 , 4% C_2H_6 (by volume), with a coflow with oxygen content of 7% and the remaining species (6% CO_2 , 12% H_2O , 74.5% N_2 by volume and other minor species, including OH) calculated with the equilibrium assumption as suggested by De et al. [20]. Additionally, flames with 8.8% and 10.9% (by mass) oxygen in the coflow and a biogas flame with 9.5% (by mass) oxygen in coflow were considered. The inlet boundary conditions for temperature and velocity were taken from experimental values measured at locations 3 mm above the jet exit. The velocity measurements were taken with Laser Doppler Anemometry (LDA) technique using a two-component, dual beam TSI-system. Temperatures were determined with a Coherent anti-Stokes Raman Spectroscopy (CARS) system described in more detail in [2,30,31]. Mean temperatures were determined from 1000 single-shot CARS spectra in each spatial position. The systematic error was estimated to be 20 K [31].

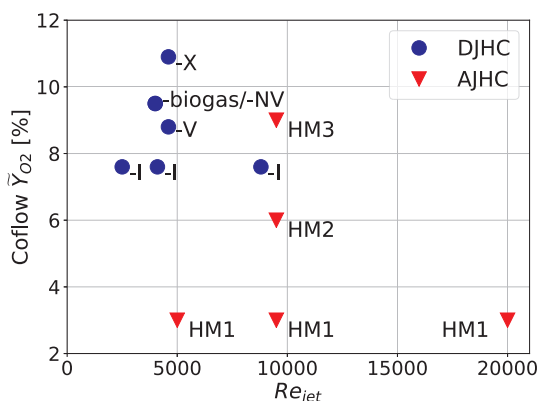


Fig. 1. Characterisation of the Adelaide and Delft Jet-in-Hot-Coflow flames: plot of jet Reynolds number vs the level of oxygen content in the coflow.

3. Numerical modelling

3.1. Turbulent combustion model

A detailed description of employed EDC variants is given in the first part of this article [1], where the generalisation of the model is introduced. In this work, the standard EDC using formulation of Magnussen [32] with $\chi = 1$ is compared with the approaches using variable reacting fraction χ [27,25], the correction proposed by Parente et al. [5] using locally modified EDC constants and the generalised formulation (see Sec. 4 of [1]). The model results are denoted as “BFM2005”, “variable χ ”, “v2016” and “generalised” respectively.

3.2. Turbulence model

The Reynolds Averaged Navier-Stokes (RANS) approach for turbulence modelling is based on time averaging and the local value decomposition into mean and fluctuation values. In RANS simulations of round jet flows it is known that the standard $k-\epsilon$ model leads to over-prediction of the jet spreading rate. This problem is usually solved using different $k-\epsilon$ model formulations or modification of its constants: $C_{\epsilon 1}$ or $C_{\epsilon 2}$. Pope [33] argued that the adjustment of the model constants is of limited value since notion of generality is lost. As an alternative, in [33] a correction was proposed which was also adopted in the present work. The modification concerns the equation for ϵ with an additional source term.

In this study, the flames are surrounded by a hot coflow. The presence of such coflow may cause some differences in comparison to simple jet flames such as a longer potential core. The length of potential core of round jets in stagnant and moving surroundings was experimentally investigated in [34]. Nathan et al. [35] reported that beside the known effect of the jet entrainment decrease due to combustion, the presence of the coflow additionally enhances this reduction. What is more, the coflow also reduces the mean spreading rate and the decay of jet centerline velocity. Additionally, in Fig. 2 it can be observed that the decay rate decreases with the decreased jet Reynolds number. As it was discussed earlier [25], it is clear that the $C_{\epsilon 1}$ correction is not applicable to (at least) the two low-Re DJHC flames. Assessment of RANS turbulence models for the JHC configuration has been also presented in many previous studies such as [10,20,13,16,22,14]. De et al. [20] showed that simulations of DJHC flames using the realizable $k-\epsilon$ model provided flow field results comparable to those obtained with the standard version. Similarly, in the work of Labahn et al. [22], the standard $k-\epsilon$ model without modifications was used. On the other hand, most of the studies on the AJHC flame employed the $C_{\epsilon 1}$ correction [10,7,5].

At the radial locations close to the nozzle, the effect of inlet boundary conditions can also play a role [36]. For example, if a uniform velocity instead of profile was taken at the fuel inlet for the AJHC, the peak radial temperature at 30 mm was shifted outside the jet. Further downstream the flame, the temperature profiles coincided. Additionally, it can be noted that the use of different computational codes

might cause differences in results, e.g. OpenFOAM seems to provide lower spreading rates than the Ansys Fluent, as it can be observed in some works using both codes [37,38,17].

3.3. Radiation

Radiation modelling in MILD regime is not a trivial problem [39]. For example, when using the Weighted-Sum-of-Grey-Gases (WSGG) model, diluted conditions will influence the WSGG coefficients. Changes in radiation intensity at different wavelengths are also expected [40]. Therefore, proper radiation modelling is needed, especially in industrial configurations. Habibi et al. [41] reported on turbulence-radiation interaction modelling and its importance, especially for the flames with lower mean temperature and stronger turbulence-chemistry interaction. However, at the same time they concluded that, compared to adiabatic results, inclusion of radiation does not alter the flame structure significantly. In general, for non-sooting laboratory jet flames radiation appears to be of less significance. Christo and Dally [10] indicated no noticeable effect on the AJHC flames with the use of Discrete Ordinates (DO) radiation model [42] in conjunction with WSGG. De et al. [20] benchmarked the DO and P1 radiation models for the DJHC flames and reported that the maximum temperature difference between the calculations with and without radiation effects was about 50 K.

In the context of the present work, we regarded radiation modelling as of secondary importance, even though we agree that considering this effect would improve the accuracy of the results in general. Having in mind the complexity of the phenomena and the relatively simple models available at hand, we did not intend to present the results obtained with the use of a doubtful radiation model, even though it would get us closer to the experimental data. Nevertheless, as mentioned above, the radiation effects in the flames considered are likely to be small. Thus, conclusions drawn from the present work are regarded to be independent of the radiation effects.

3.4. Multicomponent diffusion

In a turbulent flow, molecular diffusion is often very small compared to the turbulent diffusion. In a reacting flow, in presence of low turbulence and various species, especially hydrogen, molecular diffusion requires additional attention. Pitsch [43] investigated three possible mechanisms leading to differential diffusion effects in hydrogen fuelled flames. Among them, the occurrence of a laminar mixing layer around the turbulent potential core in the region close to the nozzle exit was found to be the most meaningful. Therefore, one might expect that including preferential diffusivities could affect the stabilisation of the flame in numerical simulations. On the other hand, Barlow et al. [44] showed that at the locations downstream the flame, turbulent stirring has a greater influence than molecular diffusion in determining the major species for the syngas flame considered. Yet, neglecting differential diffusion can lead to NO under-prediction as mentioned by Kim

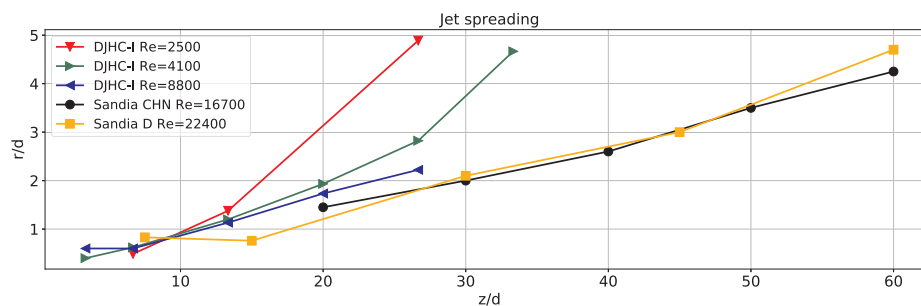


Fig. 2. Jet spreading indicated by velocity half-widths obtained from experimental data of five jet flames plotted on non-dimensional axes. Three DJHC flames with the jet Reynolds numbers of 2500, 4100 and 8800 and two flames from the TNF workshop: Sandia D ($Re = 22400$) and Sandia CHN ($Re = 16700$).

Table 1
Numerical settings for the simulations of Adelaide and Delft jet-in-hot-coflow flames.

	DJHC	AJHC
Code		OpenFOAM-2.4.0
Solver		edcSimpleSMOKEmod
Turbulence model		$k - \epsilon$ (std/Pope correction)
Combustion model		EDC
Radiation model		none
Multicomponent diffusion		yes
Molecular viscosity		Sutherland law
Pressure-velocity coupling		SIMPLE
Discretization schemes		2nd order
Fine structure reactor		PFR
Turbulent Schmidt number		0.7
Turbulent Prandtl number		1.0
Domain size	80 mm × 225 mm	120 mm × 300 mm
Mesh size	32 400	44 550
Chemical mechanism	DRM (19 sp., 84 re.)	KEE (17 sp., 58 re.)
Inlet BC (\tilde{u} , k , ϵ)	experimental data	derived expressions
Inlet BC (\tilde{T})	experimental profile	uniform exp. value
Inlet BC (\tilde{Y}_k)	uniform exp. value	uniform exp. value

and Kim [45]; nevertheless, they did not include this effect in their simulations of Sandia CHN flame. Similarly, in the computations of this flame by other authors [37,46] the lack of differential diffusivities did not lead to flame stabilisation problems. However, for the JHC

simulations in presence of large fractions of hydrogen in the fuel, the effect of multi-component molecular diffusion needs to be included. The influence of this effect on the prediction of temperature and mass fractions of major species in the mixture fraction space was presented by Christo and Dally [10]. Recently, Li et al. [16] showed that without molecular diffusion, it is not possible to capture the correct temperature peak in the radial profile 30 mm downstream the flame. This is by no means a general characteristic of jet-in-hot-coflow flames, but is strictly related to the fuel composition. In the simulations of DJHC flames with natural gas as a fuel, De et al. [20] reported the effects of differential diffusion to be small. Nevertheless, in the present study multi-component molecular diffusion was taken into account in all considered cases.

3.5. Chemical mechanisms

Modelling turbulent combustion in CFD using detailed chemical mechanism is unaffordable for real fuels. Therefore, reduced kinetic schemes are needed; yet, even then, using large mechanism is computationally very expensive. Chemists who provide kinetics models usually focus on high accuracy and generality thus new chemical mechanisms can be extremely large [47]. On the other hand, CFD engineers are always in search for a trade-off between computational cost and accuracy, to reduce the chemistry overhead in numerical simulations. In the present work, we do not focus on chemistry. For each case considered, we pick up the most convenient and previously validated

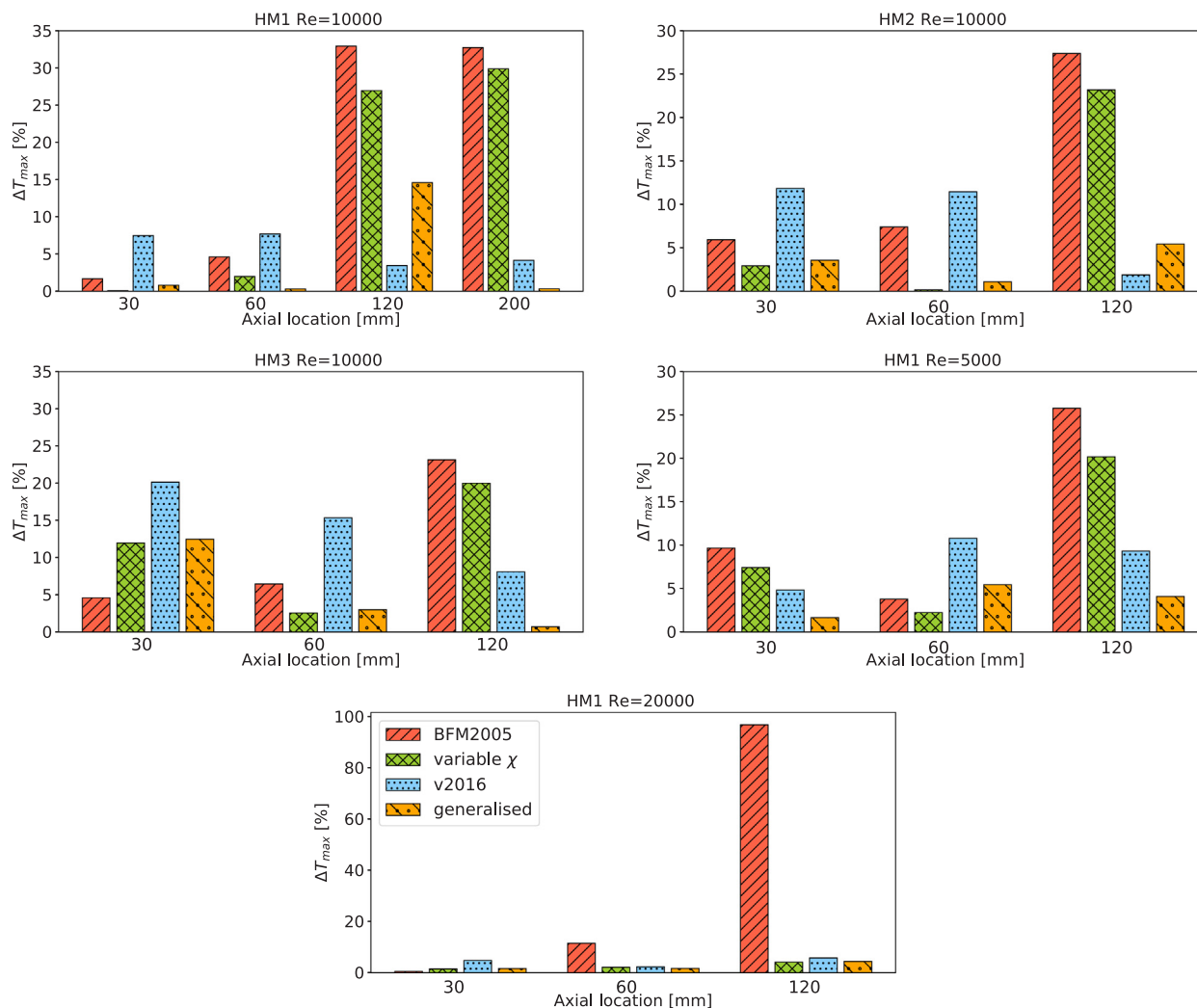


Fig. 3. Relative error of the temperature peak at selected axial location for AJHC flames.

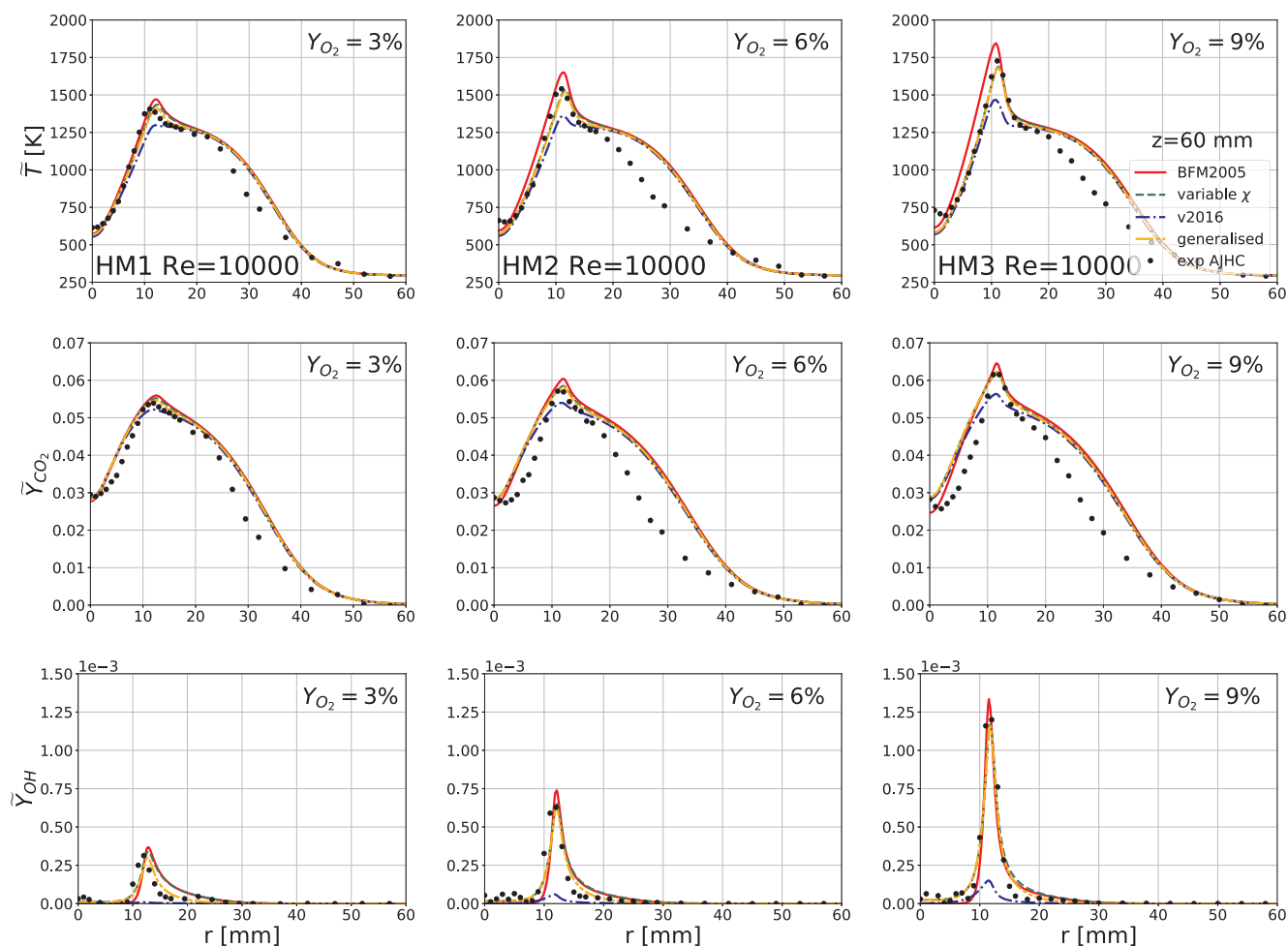


Fig. 4. Radial distributions of temperature, mass fraction of CO_2 and OH at the axial position 60 mm downstream of the nozzle for the three Adelaide JHC flames denoted as HM1, HM2 and HM3, with oxygen content in the coflow stream of 3%, 6% and 9% respectively. The jet Reynolds number was 10000 for all the flames. Comparison of simulations performed with the standard EDC with the formulation of Magnussen [32] using $\chi = 1$ (denoted as BFM2005), using variable χ approach, with locally adjusted EDC constants denoted as v2016 and with the generalised EDC.

reduced chemical mechanism. Among them, two have been used quite frequently. The reduced mechanism from GRI-1.2 known as DRM19 (19 species, 84 reactions) [48] has been used in JHC flames simulations by e.g. [6,20,21,24]. The other commonly used mechanism in AJHC flames simulations [5,12,15] is KEE (17 species, 58 reactions) [49]. Larger mechanisms have been also employed. Labahn et al. [22] used GRI-2.11 for simulations of DJHC flames. Shababian et al. [14] used GRI-3.0 and POLIMI mechanisms. Recently, Luan et al. [50] compared the GRI-3.0 with Aramco mechanisms for MILD combustion in well-stirred reactor and they reported negligible differences. Evans et al. [7] used GRI-3.0 mechanisms, stressing the high computational cost even for laboratory test cases such as AJHC flames. Li et al. [16] assessed the performances of larger mechanisms such as GRI3.0, San-Diego and POLIMI C1C3HT in their study of AJHC flames, showing marginal differences. Additionally, they reported that the simulation cost was 3.7, 4.8 and 14.3 times higher than KEE, respectively. Eventually, when one would like to use the EDC model in industrial applications the selection of reduced models would still be the most probable option.

A great advantage of the EDC model is that it can incorporate finite rate chemistry using a given chemical mechanism, be it full, detailed or reduced. This, however, means that the number of transport equations for the species mass fractions can be tremendous if detailed chemistry is used, and the CPU time might be prohibitive for industrial applications. Reaction mechanisms get more complex with the number of the carbon

atoms in the fuel. Thus, involving realistic fuels is associated with larger chemical mechanisms. From our experience, integration of the ordinary differential equations (ODE) system is responsible for ca. 65% to over 90% time consumption of each CFD time step, which makes it the most expensive process. At the same time this opens room for improvements.

Two main approaches applied dynamically can be used for that purpose: chemistry reduction and chemistry tabulation. The first approach allows CPU savings due to the reduction of the number of species in each computational cell, preserving an accuracy comparable to the original scheme. As a result one can expect to have a large number of active species in the flame region and a significantly reduced scheme in regions where only major species play a role. The second method aims to reduce the number of direct ODE integrations using tabulation, which was demonstrated by Pope [51] in the so-called In-Situ Adaptive Tabulation (ISAT) algorithm. Li et al. [24] investigated a combination of several reduction techniques coupled with the dynamic tabulation using ISAT. The approach is named as Tabulated Dynamic Adaptive Chemistry (TDAC). As validation test cases, two Delft JHC flames were simulated: one fuelled with natural Dutch gas at $Re = 4100$ and another fuelled with biogas at $Re = 4000$. Three chemical mechanisms were tested: DRM19 (19 species, 84 reactions), GRI3.0 (53 species, 325 reactions) and POLIMIC1C3HT (107 species, 2642 reactions). Five reduction models were assessed: the directed relation graph (DRG), the directed relation graph with error propagation (DRGEP), the dynamic adaptive chemistry (DAC), the elementary flux analysis (EFA) and the

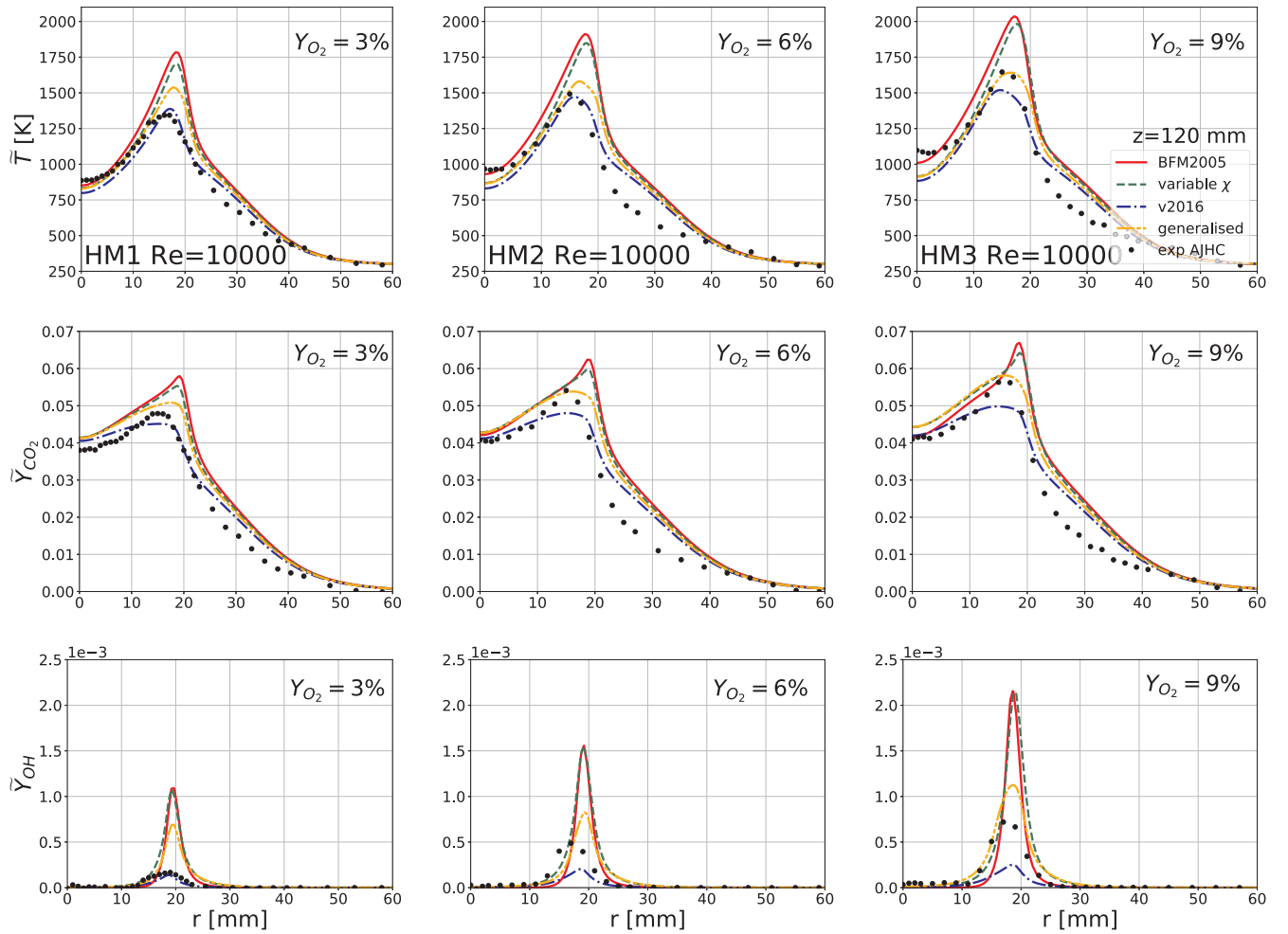


Fig. 5. Radial distributions of temperature, mass fraction of CO₂ and OH at the axial position 120 mm downstream of the nozzle for the three Adelaide JHC flames denoted as HM1, HM2 and HM3, with oxygen content in the coflow stream of 3%, 6% and 9% respectively. The jet Reynolds number was 10000 for all the flames. Comparison of simulations performed with the standard EDC with the formulation of Magnussen [32] using $\chi = 1$ (denoted as BFM2005), using variable χ approach, with locally adjusted EDC constants denoted as v2016 and with the generalised EDC.

path flux analysis (PFA). Detailed description of the TDAC algorithms is out of scope of the present work, yet the main idea of improvement in CPU time is essential for further use of the EDC model in industrial applications. The complete analysis can be found in [24] and description of the algorithms is given in [51].

Based on the work published in [24], some major conclusions and recommendations can be made: the contribution of tabulation is more important with small mechanisms, while the reduction plays a major role with large mechanisms. The following three reduction methods: DRGEP, DAC and EFA significantly outperformed the other two, DRG and PFA. Using the TDAC method provides considerable benefits for larger chemical mechanisms such as the comprehensive POLIMI1C3HT (speed-up factor over 10); using already reduced mechanisms such as DRM19, the speed-up factors are modest (1.4–2.0).

Additionally, it should be pointed out that there is some discussion on whether standard chemical mechanisms can be used for MILD combustion, as they are required to work outside the conditions used for their optimisation [52,53]. Ongoing research aims at reliable models for MILD combustion chemistry. Alternatively, existing models may be improved, e.g. Tu et al. [54]. Nevertheless, at the moment we do not see a ready answer for the usage of chemical kinetic models developed especially for MILD combustion. The standard DRM19 or KEE mechanisms proved to perform satisfactorily in previous studies on the DJHC and AJHC flames [7,16,20,21].

3.6. Inlet boundary conditions

The inlet boundary conditions for temperature and velocity profiles were taken from experimental data close to the burner exit. The turbulence kinetic energy profile was calculated from the measured axial and radial components of the Reynolds stresses, while assuming that the azimuthal component $\overline{w''w''}$ was equal to the radial $\overline{v''v''}$, as proposed by De et al. [20]:

$$k = \frac{1}{2} \overline{u''u''} + \overline{v''v''}. \quad (1)$$

The inlet profile of the mean turbulence energy dissipation rate was estimated by assuming it equal to the turbulence energy production:

$$\epsilon = -\overline{u''v''} \frac{\partial \tilde{u}}{\partial r}. \quad (2)$$

Alternatively, this method can be extended even if the Reynolds stresses are unknown, using expressions for k and ϵ derived by Lewandowski et al. [36]:

$$k = C_k d (Re)^{-\frac{1}{8}} \tilde{u} \frac{\partial \tilde{u}}{\partial r} \quad (3)$$

and

$$\epsilon = C_\epsilon d (Re)^{-\frac{1}{8}} \tilde{u} \left(\frac{\partial \tilde{u}}{\partial r} \right)^2 \quad (4)$$

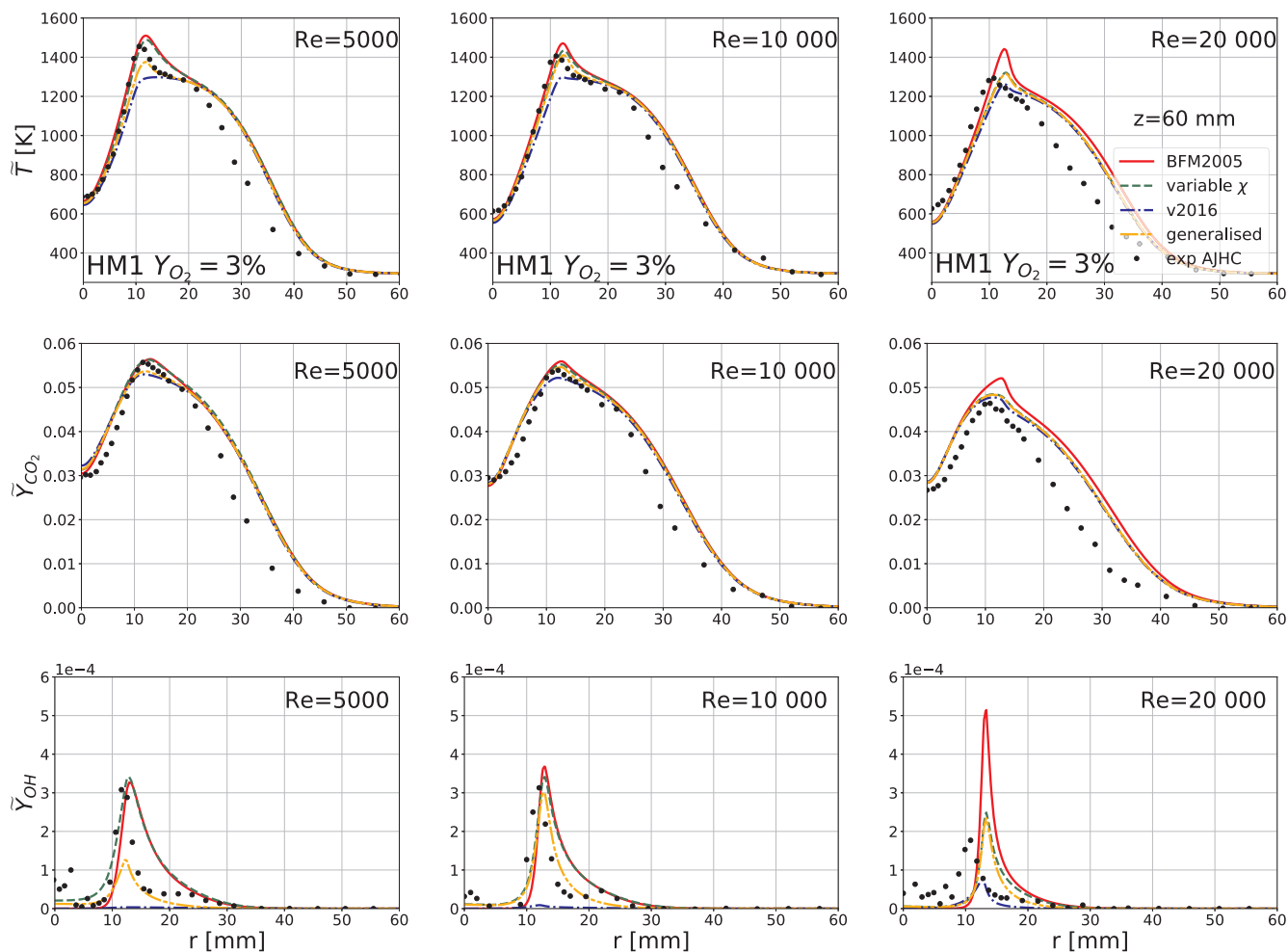


Fig. 6. Temperature, mass fraction of CO_2 and OH radial distributions at the axial position 60 mm downstream of the nozzle for the three Adelaide JHC flames denoted as HML, with the jet Reynolds number of 5000, 10 000 and 20 000 respectively. The oxygen content in the coflow stream was 3% for all the flames. Comparison of simulations performed with the standard EDC with the formulation of Magnussen [32] using $\chi = 1$ (denoted as BFM2005), using variable χ approach, with locally adjusted EDC constants denoted as v2016 and with the generalised EDC.

where $C_k = 0.025$, $C_\epsilon = 0.0075$ [36], d is the fuel pipe diameter and Re is the jet Reynolds number. For the air tunnel no detailed measurements were available, thus the constant values were used. In both burners the ambient air temperature was set to 293 K, whereas velocity was set to 0.5 m/s and 3.3 m/s for DJHC and AJHC cases, respectively.

In the simulations of AJHC burner, Christo and Dally [10] and Frassoldati et al. [13] pointed out that the numerical solution was sensitive to the turbulence level at the inlets. However, they did not have access to the experimental inlet data and had to perform cold flow simulations inside the burner [10], use a pre-inlet pipe [13] and make some adjustments of the turbulence quantities to obtain a correct jet spreading rate. Frassoldati et al. [13] and Aminian et al. [12] performed sensitivity analysis of the inlet turbulence level on the results. Variations of k of two orders of magnitude showed significant differences in the results. Evans et al. [7] pointed out that sensitivity to the inlet boundary condition, including for the turbulence intensity, was also related to the modifications of the EDC parameters. Influence of assigning different turbulence inlet conditions was also previously investigated by Merci et al. [55] who analysed different methods for determination of inlet ϵ . We have followed the suggestion of Frassoldati et al. [13] and adjusted inlet turbulence level to obtain a proper amount of oxygen diffusing from the shroud air towards the flame. We ended up with very similar results concluding that their inlet conditions are optimal. Since those values were also adopted by other researchers (e.g. [5,16,17,6]) their use also enables reliable comparison of the

simulation results with previous works. The only exception are the inlet conditions for fuel jet in AJHC burner, where profiles for k and ϵ were assigned based on Eqs. (3) and (4). This method was analysed in [36] and even though the profiles were closer to the experimental data, their impact on the non-premixed jet flames results turned out to be small. This confirmed previous observation [13,12] that the influence of coflow inlet conditions is much stronger.

3.7. Numerical settings

Simulations were run using OpenFOAM code [56] with the *OpenSMOKE* library [57] and the modified steady solver *edcSimpleSMOKE* [58], using SIMPLE algorithm for the pressure-velocity coupling. A two-dimensional axisymmetric configuration was used. For the DJHC flames the computational domain extended 225 mm in axial and 80 mm in radial direction, whereas for the AJHC flames the domain size was 300×120 mm². A grid independence study was performed for both cases with the refinement ratio between the meshes equal to 1.5. Additionally, a method based on the Richardson extrapolation was applied to evaluate the Grid Convergence Index (GCI) with a safety factor set to 1.25. The mesh with the mean GCI < 2% for each radial location was assumed to be fine enough. All the details of numerical simulation setup can be found in Table 1. It should be pointed out that in the current simulation, a turbulent Prandtl number equal to 1.0 was used. According to the literature, for non-isothermal round jets the value should

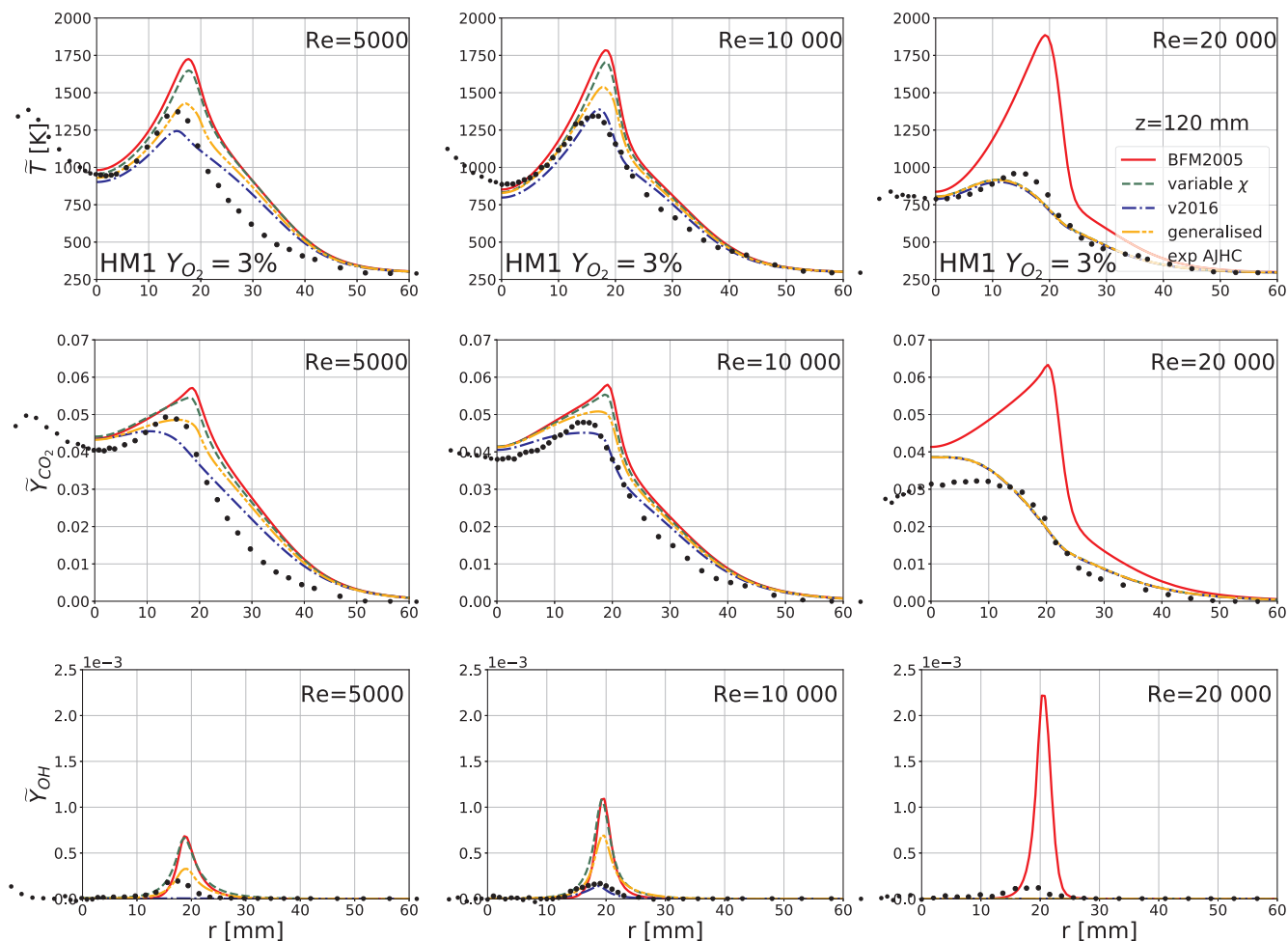


Fig. 7. Temperature, mass fraction of CO₂ and OH radial distributions at the axial position 120 mm downstream of the nozzle for the three Adelaide JHC flames denoted as HM1, with the jet Reynolds number of 5000, 10 000 and 20 000 respectively. The oxygen content in the coflow stream was 3% for all the flames. Comparison of simulations performed with the standard EDC with the formulation of Magnussen [32] using $\chi = 1$ (denoted as BFM2005), using variable χ approach, with locally adjusted EDC constants denoted as v2016 and with the generalised EDC.

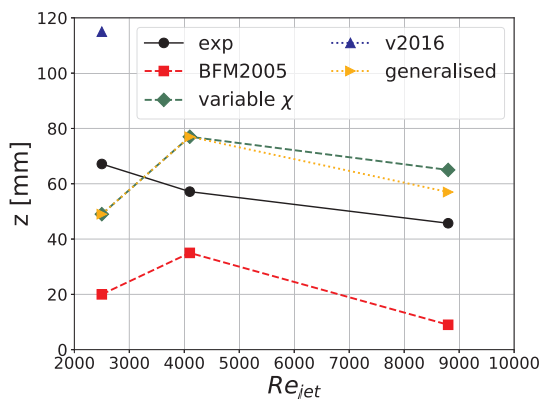


Fig. 8. Lift-off heights for the three DJHC-I flames with the same level of dilution but three different jet Reynolds numbers. The lift-off heights were estimated based on the OH radicals as the reaction zone indicator.

be somehow lower, e.g. 0.81 [59]. Recently, for the AJHC flames, Li et al. [16] compared temperature profiles obtained using $Pr_t = 1.0$ and $Pr_t = 0.85$ concluding that it barely influenced the results. On the other hand, one can try to use variable turbulent Schmidt and Prandtl number modelling [60].

4. Validation results

The study was performed on five Adelaide flames and seven Delft JHC flames. Selected data will be shown for radial distributions comparing trends observed for various jet Reynolds numbers and co-flow oxygen levels.

4.1. Adelaide Jet-in-Hot-Coflow

To visualise effect of different EDC variants in the AJHC flames, Fig. 3 presents relative errors of the maximum temperature peaks at available radial temperature distributions. A clear advantage of the generalised EDC can be easily noticed, with the exception of HM1 flame ($Re = 10000$) at 120 mm downstream the jet exit plane. The data presented in Fig. 3 for the flame at high Reynolds number $Re = 20000$ show extremely high error at the location 120 mm for the standard EDC and very small deviations in other locations for all the model variants. However, it should not be understood as good performance of the employed modifications, since all of them led to flame extinction.

The results are presented in figures composed of nine plots in three rows and columns. In Figs. 4 and 5, the columns indicate cases with different level of dilution (3%, 6% and 9% of oxygen in the coflow), whereas in the rows temperature, mass fractions of carbon dioxide and the hydroxyl radical are presented. It is important to note that for AJHC, experimental data for species mass fractions are available

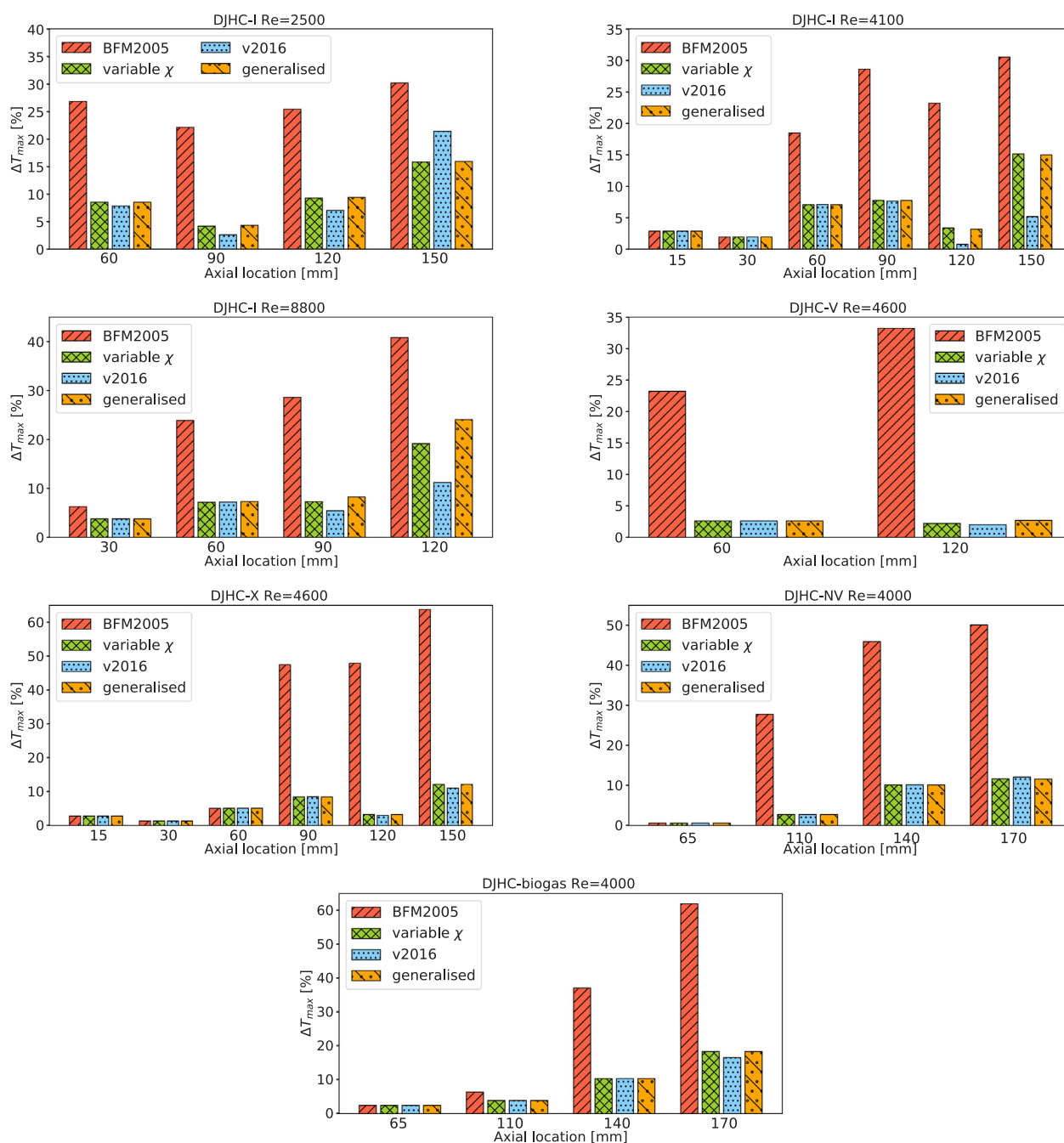


Fig. 9. Relative error for the prediction of the temperature peak at selected axial locations for seven DJHC flames.

enabling a quantitative comparison of numerical results. In Figs. 6 and 7 the results of the same set of scalars are presented for the flame HM1 with 3% oxygen in the coflow at three different Reynolds numbers 5000, 10000 and 20000.

In Fig. 4, it is very clear that the temperature, CO₂ and OH mass fractions are only slightly over-predicted by the standard EDC at 60 mm downstream of the nozzle, for all three flames. However, modification “v2016” with locally variable EDC constants leads to an under prediction of the temperature peaks by 200–250 K. For HM1, this variant does not capture the characteristic temperature peak, whereas for HM2 and HM3 flames the predicted peak is too low. The relative discrepancy is even larger for the OH radical predictions. The approaches with variable χ and the generalised EDC give nearly the same results improving the prediction of standard EDC and leading to a perfect fit with the experimental measurements for all the scalars.

The situation changes if we look at the results further downstream at $x = 120$ mm presented in Fig. 5. Using the standard EDC, a high over-prediction is observed for all scalars and the variable χ does not remedy this deterioration at all. The model version “v2016” performs much better at this location. For HM1 flame an almost perfect prediction of the temperature and OH is obtained, with only a small under-prediction of CO₂ peak value. For HM2, the temperature distribution is in a very good agreement with the experimental data but the mass fractions of CO₂ and OH are under-predicted. For HM3, the under-prediction is observed for all the presented data. Compared to all other model variants, the generalised EDC provides reasonably good agreement with the experimental data. However, the temperature peak is over-predicted by 15% for HM1, while the agreement is excellent for the other two flames. Consequently, CO₂ is over-estimated only for the case with 3% of oxygen content in the coflow, otherwise the matching was very

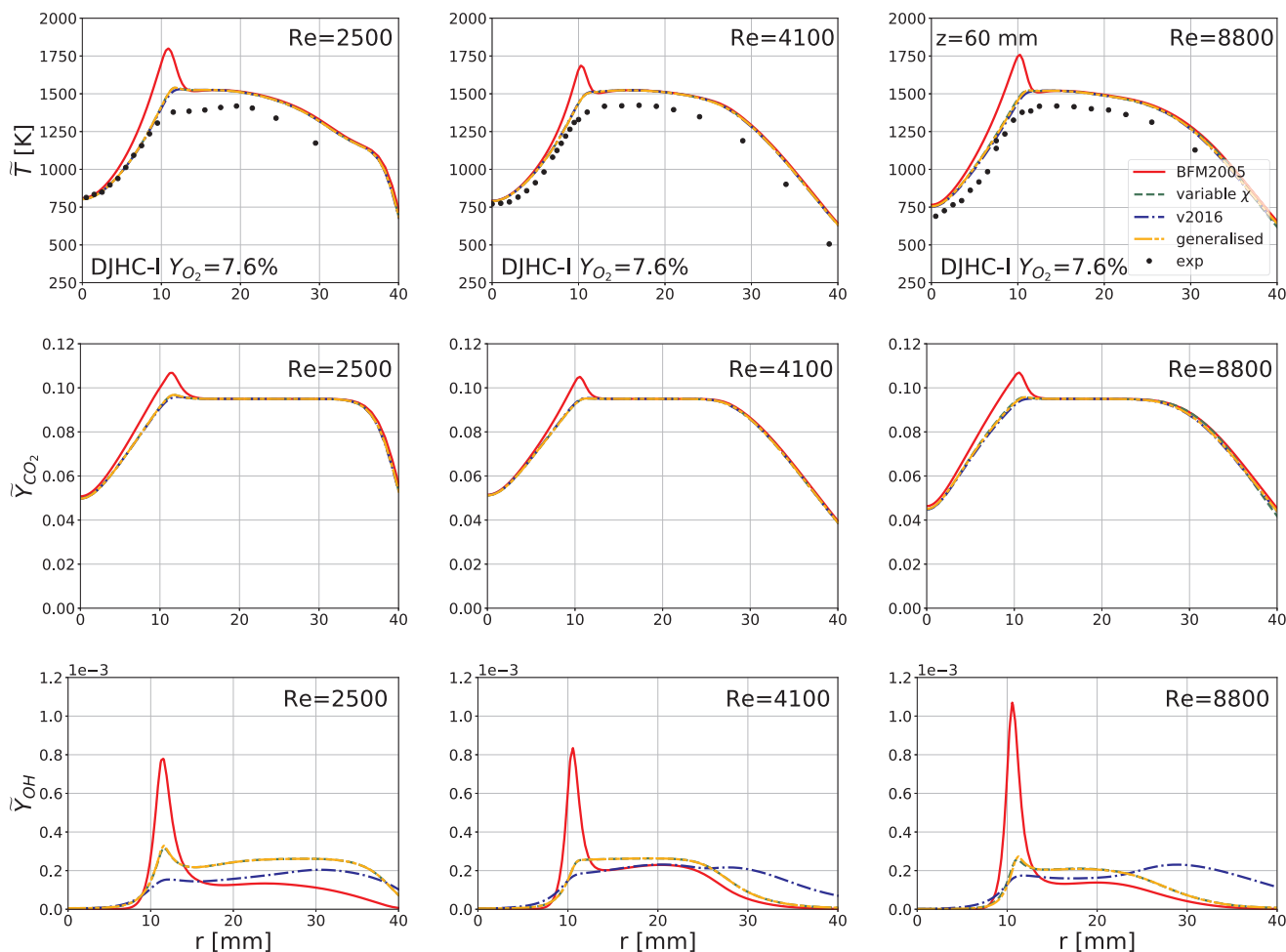


Fig. 10. Temperature, mass fraction of CO_2 and OH radial distributions 60 mm downstream of the nozzle for the three DJHC-I flames with jet Reynolds numbers 2500, 4100 and 8800. Comparison of simulations performed with the standard EDC using $\chi = 1$ (denoted as BFM2005), the variable χ approach, the locally adjusted constants (v2016) and the generalised EDC.

satisfactory. The maximum OH mass fraction value is higher in all three cases with relative error decreasing with increasing the oxygen content in the coflow. Overall, as far as the dilution level is considered, the generalised EDC indeed provides the most satisfactory results across the investigated configurations.

For the flames with different jet Reynolds number at location 60 mm downstream the jet plane (see Fig. 6), the temperature under-prediction with “v2016” is observed for low and medium Reynolds number cases, where almost no OH is present. For high Reynolds number case, the temperature and CO_2 peaks are predicted quite well with some shift toward the outer side of the jet. The hydroxyl radical peak is predicted at the correct location, yet twice too small. The standard EDC and with the use of variable reacting fraction provide very similar results for low and medium Reynolds number cases, with relatively good agreement with the experimental data. At high Reynolds number, the standard EDC over-predicts peaks of all three presented scalars, which are clearly improved with the variable χ and the generalised EDC. Especially, the calculated maximum OH value matches the experiment very well, yet also with some shift outside the jet axis indicating higher jet spreading. For the low Reynolds number case, the generalised EDC provides a lower temperature peak and under-estimates the OH mass fraction.

The situation is very different downstream the three flames at $x = 120$ mm, as presented in Fig. 7. For the low Reynolds number flame, only the generalised EDC provides good results for all scalars. As previously mentioned, the standard EDC and the variable χ formulation

over-estimate all the scalars of interest. On the other hand, the model with locally variable EDC constants under-estimates temperature, CO_2 mass fractions and provides no OH peak at all. The same model for medium Reynolds number (HM1 case), provides very good agreement with the experiment at downstream locations. However, for the high Reynolds number flame, the numerical results are far from satisfactory. The standard EDC highly overestimates all the scalars, whereas the three investigated EDC corrections lead to flame extinction. For the low Reynolds number case with “v2016”, flame re-ignition is observed further downstream; the same is not observed for the high Reynolds number case, whatever the correction. The extinction of flame HM1 at $Re = 20000$ with “v2016” model was also observed and discussed by Parente et al. [5]. It was reported that due to the increased jet velocity, experimental data showed a strong temperature reduction which was caused by partial extinction of the flame. They showed instantaneous temperature results as a function of mixture fraction in Fig. 6 in [5] for this case where the amount of partial extinction and re-ignition was very high, which was indicated by large scatter of the data. To conclude, using RANS-EDC approach one can get either a stable flame, with significant temperature over-prediction, or flame extinction, indicating that the model is not adequate for this particular case. Yet, this is not necessarily related to EDC itself but in general to the RANS framework. It is believed [5] that a more sophisticated turbulence approach could deal with this problem.

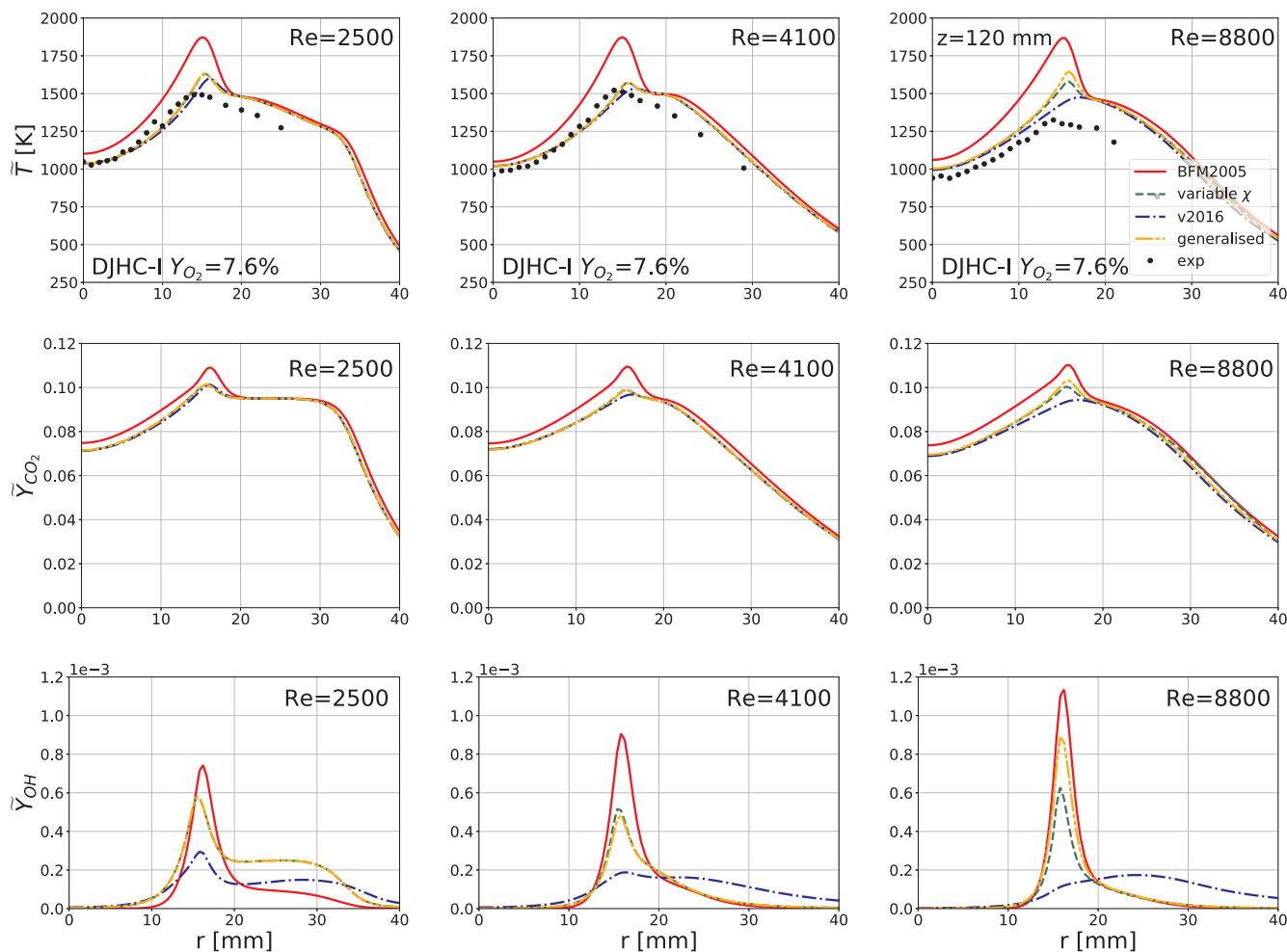


Fig. 11. Temperature, mass fraction of CO_2 and OH radial distributions 120 mm downstream of the nozzle for the three DJHC-I flames with jet Reynolds numbers 2500, 4100 and 8800. Comparison of simulations performed with the standard EDC using $\chi = 1$ (denoted as BFM2005), the variable χ approach, the locally adjusted constants (v2016) and the generalised EDC.

4.2. Delft Jet-in-Hot-Coflow

In Fig. 8 the lift-off height predictions with the four modelling approaches are presented for the three DJHC flames. The lift-off heights were defined as the axial distances from the nozzle where the mass fraction of OH increased over 2.8×10^{-4} . This value corresponds to the amount of OH in the coflow stream, and it is then regarded as a threshold for the OH radical produced in the reaction zone. Therefore, such definition was considered to compare the numerical results with the experimental RMS values of OH-fluorescence from Oldenhof et al. [2]. At the same time, such definition suffers from significant uncertainty and the presented results have a rather qualitative character. Some differences can be observed between the results presented in [25] and Fig. 8; this comes from the use of slightly different numerical setup, yet the characteristic behaviour is preserved. A first comment should be made for the approach v2016, for which the amount of OH above the stated value was observed only for the low Reynolds number case. For other DJHC flames, the OH production was negligibly small indicating flame extinction. For the low and medium Reynolds number case, the generalised model provided the same lift-off height as the variable χ approach. However, for the flame at $Re = 8800$, the generalised model gave a lower lift-off height than the variable χ alone, which is in better agreement with the experimental data. Nevertheless, the experimental trend of the lift-off height decrease with increasing jet Reynolds number is captured only for the medium and high Reynolds number cases. In all the simulations without *ad hoc* adjusted parameters, the lift-off height

for the low Reynolds number flame was smaller than for the flame at $Re = 4100$. This effect can be also observed in Figs. 10 and 11, where the OH peak is slightly higher for the flame at $Re = 2500$ than at $Re = 4100$, using the model correction.

On the other hand, it should be pointed out that the effect of lower lift-off height for the higher Reynolds number jets is associated with the higher entrainment in combination with the positive radial temperature gradient in the coflow [2]. Medwell et al. [61] also observed that the lift-off height decreased with the jet velocity in AJHC flames. They mentioned that this trend is likely related to shorter ignition delay caused by the increased mixing at the shear layer. Therefore, capturing this effect requires an appropriate choice of the turbulence-chemistry interaction closure and of the turbulence model, to get correct mixing of the two streams.

In Fig. 9 relative errors of the temperature peaks of all seven DJHC flames are shown for all the axial locations where the experimental data were available. It is very clear that all three modifications considerably reduced the error in comparison to standard EDC. Since DJHC flames do not show sharp temperature peak, any modifications reducing the over-prediction exhibited by standard EDC showed similar relative errors for the maximum temperature. To better quantify performance of the applied modifications, a closer look into the flame structure is needed.

The four versions of the EDC are compared at two different axial locations: 60 mm and 120 mm downstream the nozzle. Figs. 10–14 are composed of nine plots in three rows and columns. The first row shows

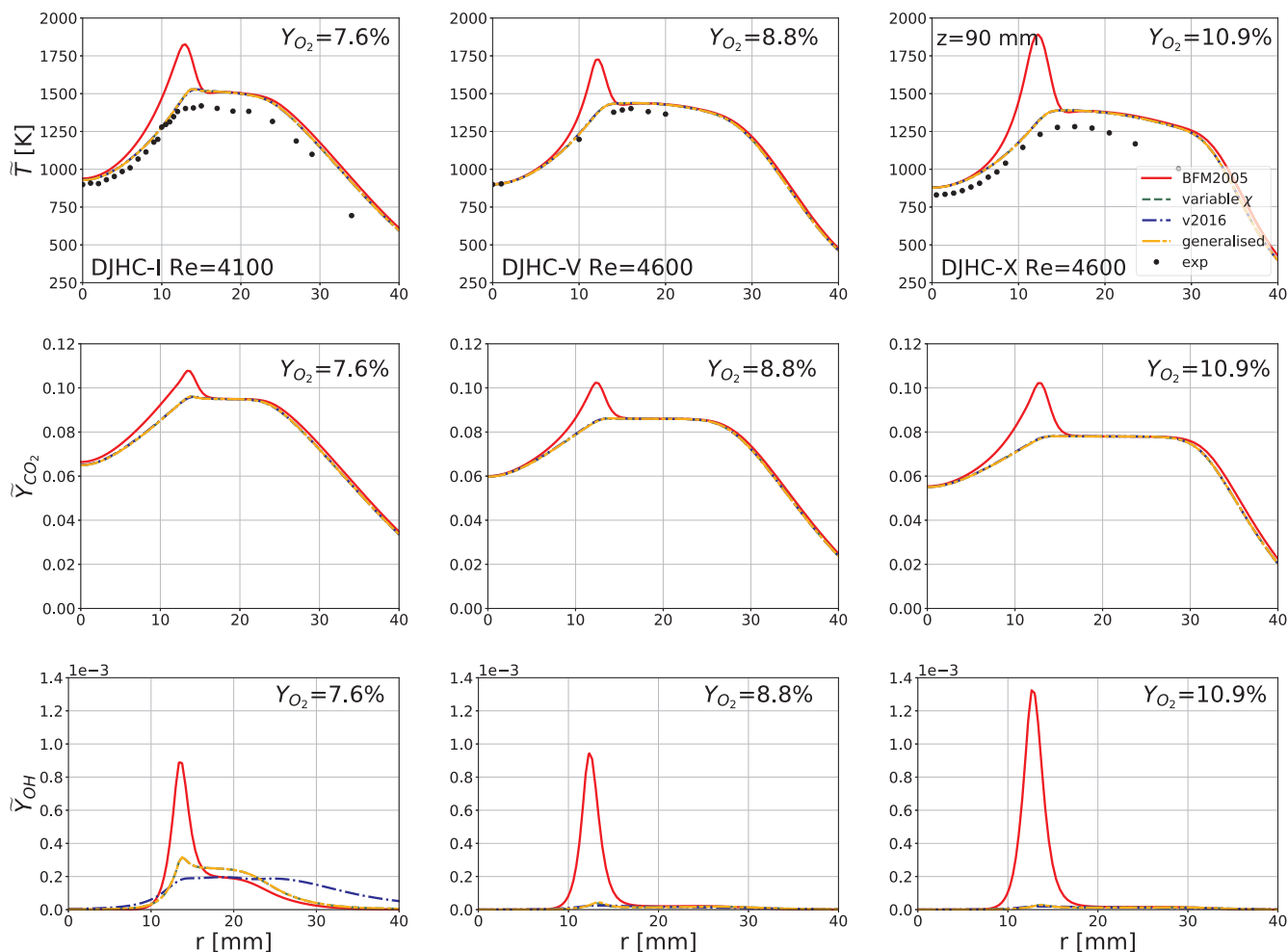


Fig. 12. Temperature, mass fraction of CO_2 and OH radial distributions 90 mm downstream of the nozzle for the three DJHC flames denoted as I, V and X with oxygen content in the coflow stream of 7.6%, 8.8% and 10.9% respectively. Comparison of simulations performed with the standard EDC using $\chi = 1$ (denoted as BFM2005), the variable χ approach, the locally adjusted constants (v2016) and the generalised EDC.

temperature results, whereas the second and the third rows present the mass fractions of carbon dioxide and hydroxyl radical, respectively. Each column indicates a different case. Accordingly, Figs. 10 and 11 show results of flames simulations with the same level of dilution $Y_{\text{O}_2} = 7.6\%$, but with three different jet Reynolds numbers (2500, 4100 and 8800). Figs. 12 and 13 show results for flames with approximately the same jet Reynolds number 4100–4600, but with different level of oxygen dilution (7.6%, 8.8% and 10.9% Y_{O_2} in the coflow stream). In Fig. 14 each column shows the results from different EDC variant.

At the location close to the nozzle all the corrections gave nearly the same results for temperature and CO_2 predictions, reducing all peak values as seen in Fig. 10. However, some differences can be observed for minor species such as OH, for which the model “v2016” predicts lower OH values than “variable χ ” and the generalised approach. In the upstream part of the jet, due to low Re_r conditions, the generalised approach uses standard set of constants and the reduced value of χ , as indicated by the identical results obtained with the two modifications. Further downstream at 120 mm (see Fig. 11) a discrepancy between the two corrections and the “v2016” model can be noticed also for major species and temperature. However, for the DJHC case at $Re = 2500$ the generalised approach still works as the variable χ approach, because of the low turbulence level. Moreover, the differences in the results are more pronounced at $Re = 8800$ than at $Re = 4100$. For higher Reynolds number, where the differences between the results are more pronounced the generalised EDC leads to slightly higher temperature, CO_2 and OH predictions than the variable χ approach alone. When it comes

to OH mass fraction, the “variable χ ” approach predicts a marked peak at the downstream locations for all three flames, whereas “v2016” predicts a peak only for the low Reynolds number case. Further downstream, the latter model predicts even lower OH values and a decrease in temperature. This indicates flame extinction, as suggested by the temperature field for “v2016”. Thus, for the conditions studied here only the “variable χ ” and generalised EDC approaches provide physically consistent results, compared to the experimental data. It should be also pointed out that downstream of the high Reynolds number flame, temperature predictions are clearly off. It should be clarified that a temperature decrease was observed experimentally, due to the cooling effect of cold, ambient air entrainment [2]. The latter is not captured by RANS simulations, indicating that the observed discrepancy should be rather ascribed to turbulence modelling.

In Figs. 12 and 13, the model response to the change in the level of coflow dilution is investigated. Firstly, it is evident that all three modifications correct the high temperature peak predicted by standard EDC. It is also noticeable that for the flames V and X, the corrections lead to trace amount of OH radicals. This is in agreement with the experimental observation that the lift-off heights are much higher than for case I, and that in flame X the lift-off height exceeds the measurement area. Thus, the results shown for the latter flame present the non-reacting part of the jet. However, further downstream at locations $x > 180$ mm, a clear flame brush is observed using the variable χ approach, not captured with the “v2016” correction, which predicts a very small production of OH ($\tilde{Y}_{\text{OH}} \approx 10^{-5}$), indicating flame extinction.

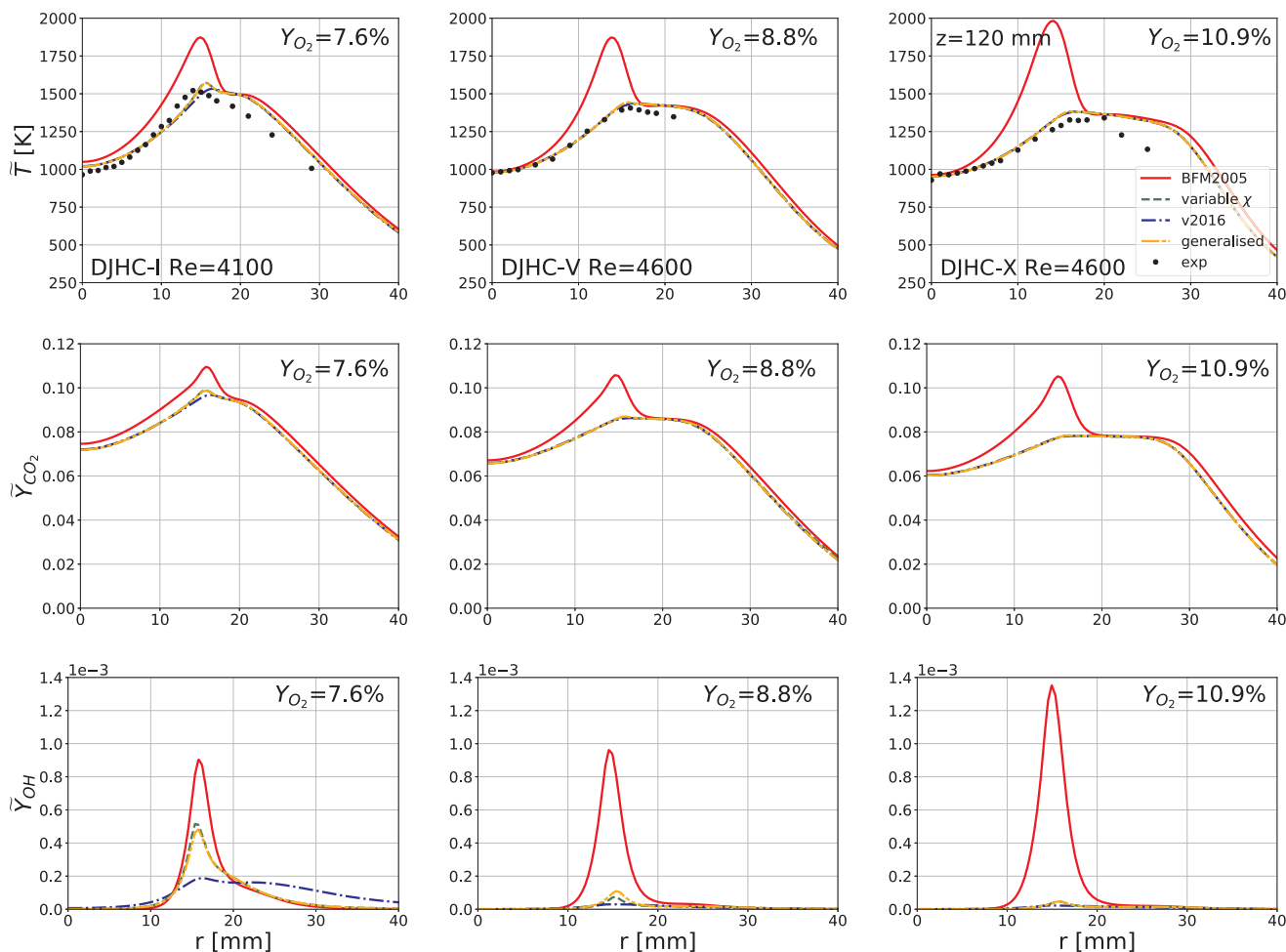


Fig. 13. Temperature, mass fraction of CO_2 and OH radial distributions 120 mm downstream of the nozzle for the three DJHC flames denoted as I, V and X with oxygen content in the coflow stream of 7.6%, 8.8% and 10.9% respectively. Comparison of simulations performed with the standard EDC using $\chi = 1$ (denoted as BFM2005), the variable χ approach, the locally adjusted constants (v2016) and the generalised EDC.

Temperature data for the three flames show slightly higher values when the oxygen content in the coflow is lower. This effect is also qualitatively captured by the variable χ simulations. This is not necessarily related to larger lift-off heights but rather to higher temperatures in the coflow streams for the flames with lower oxygen level. Due to the large lift-off heights of those flames, and different coflow temperatures, it is challenging to make an adequate comparison to capture the effect of dilution.

In Fig. 14 the data from the two flames are presented in single plots to make a distinct comparison between the flames under the same flow conditions but with different fuel. Numerical results obtained with the standard EDC are compared to the experimental data at location $z = 140$ mm downstream of the nozzle. At $z = 65$ mm (not shown) no temperature rise is observed and the data for both flames are superimposed. Note that the differences in CO_2 distribution between the two flames simply indicate a different fuel composition. The standard EDC shows high temperature over-prediction for both cases. The two considered corrections improve the predictions, yet they provide very similar results for temperature and carbon dioxide. However, for OH mass fraction distribution the generalised EDC produces sharper peaks than the “v2016” correction. Further downstream, the “v2016” correction predicts a very modest peak indicating flame extinction (see Fig. 15). For the standard EDC results it is interesting to note that the temperature peak is higher for the natural gas, whereas the OH peak is higher for the biogas flame. Different results are obtained using the various corrections, since higher OH values are obtained for natural

gas. Yet their values are one order of magnitude lower than the results obtained with standard EDC. However, no quantitative comparison is possible without experimental data.

The results for cases V, X, NV and biogas presented in Figs. 12–14 reveal very similar behaviour, since all the corrections provide almost the same results at the locations where the experimental data are available. The lift-off heights for those flames are large, and for X flame the lift-off height exceeds the measurement area. At the same time, it should be pointed out that high peak values for all scalars predicted by the standard EDC are corrected with all the modified EDC variants. In Fig. 15, the results for the flames V, X and biogas are presented at the location $x = 220$ mm, without comparison with the experiment. These results indicate that the differences between different model variants become visible at this location. This suggests that, the flame develops much further downstream the jet exit plane in contrast to the I flame series. Moreover, in Fig. 15 an additional line for the simulation results without chemical reaction is presented. It is visible that the flame simulated with the correction “v2016” exhibits symptoms of extinction since the results almost coincide with the non-reacting simulation.

5. Conclusions

The Eddy Dissipation Concept (EDC) for turbulence-chemistry interaction was assessed in the flames issuing from two JHC configurations. The EDC closure is widely adopted in practice and it represents a promising model for MILD combustion simulations. The model

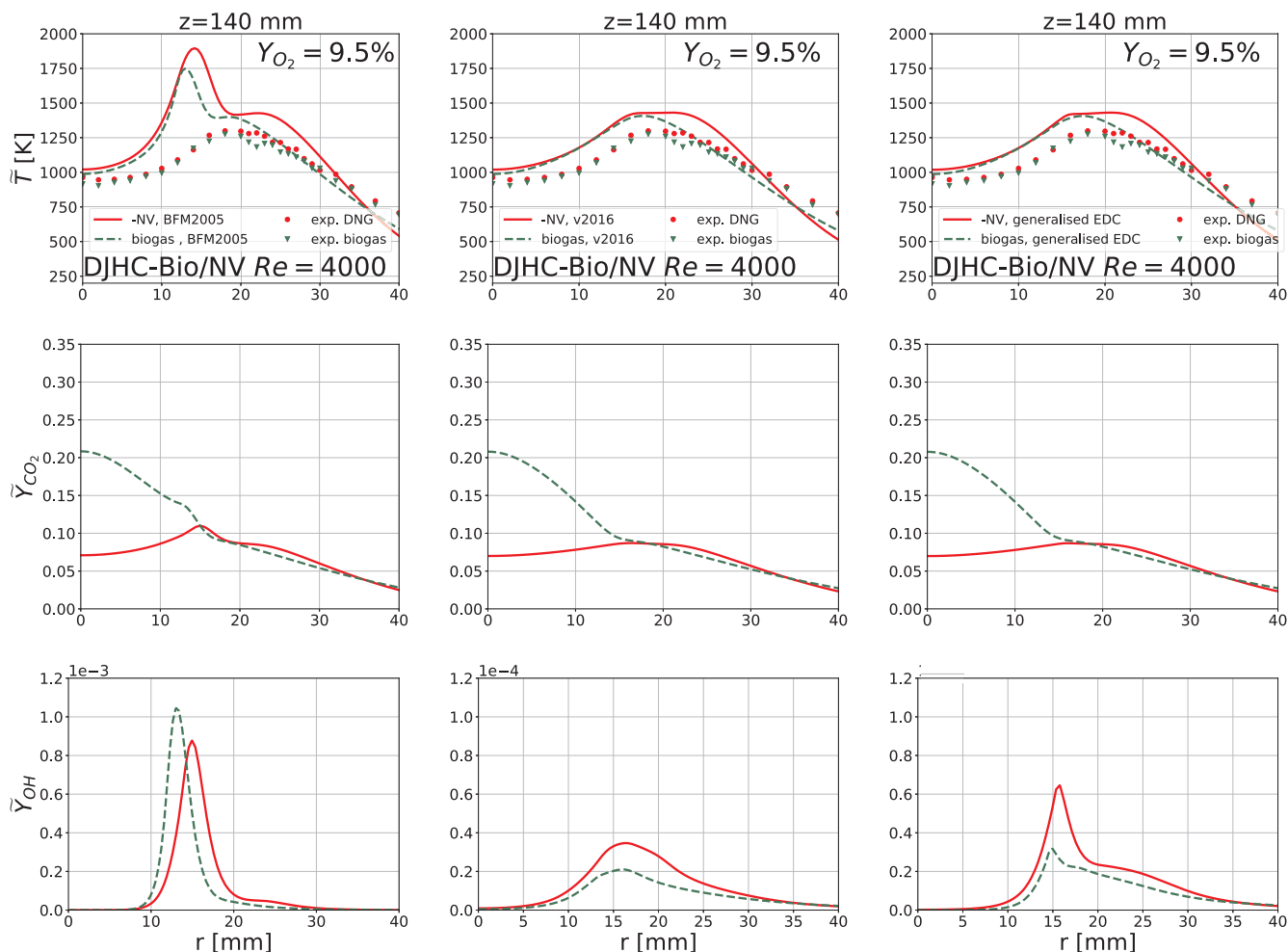


Fig. 14. Temperature, mass fraction of CO_2 and OH radial distributions 140 mm downstream of the nozzle for the two DJHC flames fuelled with biogas and Dutch natural gas was at $Re = 4000$ and 9.5% of oxygen in the coflow stream. The first column shows the results obtained with the standard EDC using $\chi = 1$ (denoted as BFM2005), the second column presents the correction with locally adjusted constants (v2016) and the third column shows results with the generalised EDC. Note that the scale range for the OH mass fraction obtained with standard EDC is up to $1.2 \cdot 10^{-3}$, whereas for the corrected cases it is up to $1.2 \cdot 10^{-4}$.

generalization presented in the first part of this study [1] was validated and compared with previous modifications. It is important to note that the validation process was based on a relatively large number of experimental cases, characterised by various levels of dilution and turbulence, as well as by different fuels. To the best of our knowledge, such a thorough validation process was not reported in previous studies aiming at assessing the performance of EDC-based models. The proposed generalised model (see Sec. 4 of [1]) considerably improves predictions with respect to the standard model for almost all the considered flames. Even though the predictions of the other EDC variants provided better results in some regions, only the generalised approach provided consistently good results in all investigated conditions, proving its generality and reliability. The proposed generalised EDC model is not case-dependent, it smoothly switches to the standard model for classical combustion conditions and adjusts to the local Damköhler and turbulence Reynolds numbers.

The main findings of the present work are now highlighted:

- a new method for turbulence inlet boundary conditions [36] was successfully employed for AJHC flames;
- the higher jet spreading rate of low Reynolds number JHC flames was shown to deviate from self-similarity of the round jets and relevant RANS turbulence modelling approaches were discussed;
- two recent modifications to the EDC based on variable reacting fraction [25] and locally modified constants [5] were assessed for

numerous JHC flames emulating MILD conditions. Both corrections led to improved results, yet none of them proved to perform satisfactorily for all investigated cases;

- the impact of the variable reacting fraction approach becomes noticeable only at low Reynolds number conditions;
- the new generalised EDC approach presented in [1] was validated on a wide range of operating conditions represented by twelve JHC flames from Delft and Adelaide proving its accuracy, versatility and robustness.

The proposed approach adjusts EDC parameters to the local flow conditions and does not add much complexity from the user point of view, thus it can serve as a convenient “plug-and-play” engineering tool.

A natural continuation of the present work would be, e.g. a computation of full-fledged combustion chamber operating in MILD regime including heat transfer and large scale recirculation. Applying the conclusions drawn from the Jet-in-Jot-Coflow flames onto industrial MILD combustion burners should be preceded by a careful analysis [30]. This circumspection comes from differences in JHC flames structure compared to industrial burners, where strong turbulent strain plays an important role. It should be pointed out, though, that we have captured the reaction zone in the case of Delft flames at extremely low Reynolds number conditions and properly modelled the mean reaction rate with the use of variable reacting fraction approach. The model performed well also for the Adelaide flames, which are characterised by

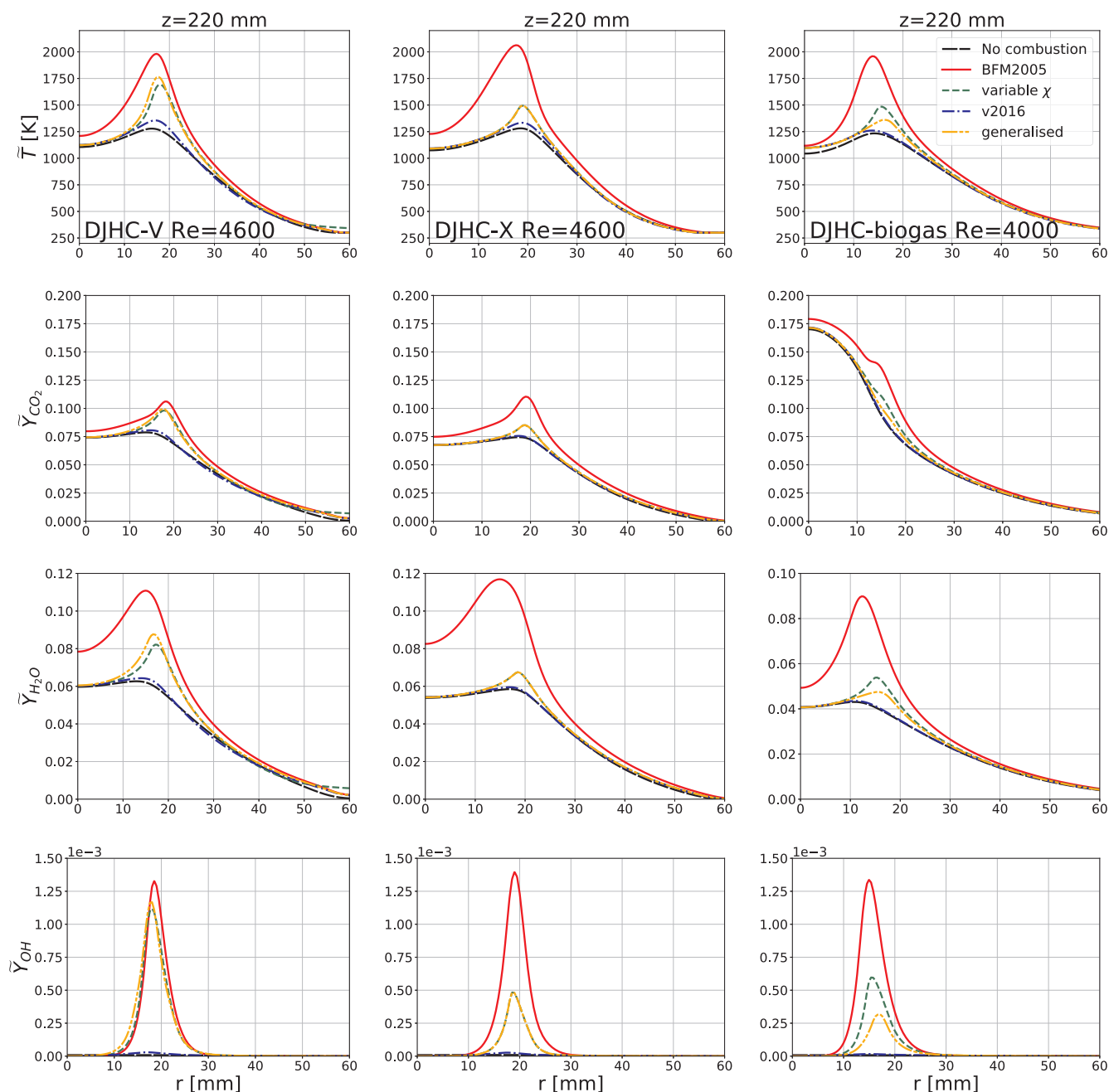


Fig. 15. Numerical simulation results at the location $x = 220$ mm downstream the jet exit plane for the DJHC flame V, X and biogas: distributions of temperature, mass fraction of CO_2 , H_2O and OH . Comparison of simulations performed with: (i) chemical reaction turned off, (ii) the standard EDC with $\chi = 1$ (BFM2005), (iii) variable χ , (iv) locally adjusted EDC constants (v2016), (v) proposed generalised model. No experimental data available at this location.

higher Reynolds numbers in the reaction zone. Future works could also include more sophisticated definitions of the reacting fraction, possibly dictated by high-fidelity DNS data. Different approaches for chemical time scale estimation may also help to capture some effects and improve the prediction, yet within the model framework and limits introduced in the first part of the study [1].

CRediT authorship contribution statement

Michał T. Lewandowski: Conceptualization, Methodology, Validation, Visualization, Writing - original draft. **Zhiyi Li:** Software. **Alessandro Parente:** Conceptualization, Supervision, Writing - review & editing. **Jacek Pozorski:** Project administration, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

We are indebted to Professor Dirk Roekaerts at TU Delft (The Netherlands) for his courtesy to share the experimental data of DJHC flames. The AJHC experimental data were provided by Professor Bassam Dally at University of Adelaide (Australia). This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme

under grant agreement No 714605. The collaboration was enabled by a bilateral research mobility project of PAN (Poland) and F.R.S.-FNRS (Belgium) entitled “Numerical and experimental investigations of MILD combustion regime” (2017–2019). Dissemination of the results was supported by COST Action CM1404 - SMARTCATs. Calculations were carried out at the Academic Computer Centre in Gdańsk (Poland).

References

- [1] Lewandowski MT, Parente A, Pozorski J. Generalised Eddy Dissipation Concept for MILD combustion regime at low local Reynolds and Damköhler numbers. Part 1: model framework development. *Fuel* 2020 [in press].
- [2] Oldenhof E, Tummers MJ, van Veen EH, Roekaerts DJEM. Role of entrainment in the stabilisation of jet-in-hot-coflow flames. *Combust Flame* 2011;158:1553–63.
- [3] Dally BB, Karpets AN, Barlow RS. Structure of turbulent non-premixed jet flames in a diluted hot coflow. *Proc Combust Inst* 2002;29:1147–54.
- [4] Perpignan AAV, Rao AG, Roekaerts DJEM. Flameless combustion and its potential towards gas turbines. *Prog Energy Combust Sci* 2018;69:28–62.
- [5] Parente A, Malik MR, Cantino F, Cuoci A, Dally BB. Extension of the Eddy Dissipation Concept for turbulence/chemistry interactions to MILD combustion. *Fuel* 2016;163:98–111.
- [6] Mardani A. Optimization of the Eddy Dissipation Concept (EDC) model for turbulence-chemistry interactions under hot diluted combustion of CH₄/H₂. *Fuel* 2017;191:114–29.
- [7] Evans MJ, Medwell PR, Tian ZF. Modeling lifted jet flames in a heated coflow using and optimized Eddy Dissipation Concept model. *Combust Sci Technol* 2015;187:1093–109.
- [8] Chen Z, Reddy V, Ruan S, Doan NAK, Roberts WL, Swaminathan N. Simulation of MILD combustion using perfectly stirred reactor model. *Proc Combust Inst* 2017;36:4279–86.
- [9] Lee J, Jeon S, Kim Y. Multi-environment probability density function approach for turbulent CH₄/H₂ flames under the MILD combustion condition. *Combust Flame* 2015;162:1464–76.
- [10] Christo FC, Dally BB. Modeling turbulent reacting jets issuing into a hot and diluted coflow. *Combust Flame* 2005;142:117–29.
- [11] Aminian J, Galletti C, Shahhosseini S, Tognotti L. Numerical investigation of a MILD combustion burner: analysis of mixing field, chemical kinetics and turbulence-chemistry interaction. *Flow Turb Combust* 2012;88:597–623.
- [12] Aminian J, Galletti C, Shahhosseini S, Tognotti L. Key modeling issues in prediction of minor species in diluted-preheated combustion conditions. *Appl Therm Eng* 2011;31:3287–300.
- [13] Frassoldati A, Sharma P, Cuoci A, Faravelli T, Ranzi E. Kinetic and fluid dynamics modeling of methane/hydrogen jet flames in diluted coflow. *Appl Therm Eng* 2010;30:376–82.
- [14] Shabaniyan SR, Medwell PR, Rahimi M, Frassoldati A, Cuoci A. Kinetic and fluid dynamic modeling of ethylene jet flames in diluted and heated oxidant stream combustion conditions. *Appl Therm Eng* 2013;52(2):538–54.
- [15] Aminian J, Galletti C, Tognotti L. Extended EDC local extinction model accounting finite-rate chemistry for MILD combustion. *Fuel* 2016;165:123–33.
- [16] Li Z, Cuoci A, Sadiki A, Parente A. Comprehensive numerical study of the Adelaide Jet in Hot-Coflow burner by means of RANS and detailed chemistry. *Energy* 2017;139:555–70.
- [17] Li Z, Ferrarotti M, Cuoci A, Parente A. Finite-rate chemistry modelling of non-conventional combustion regimes using a partially-stirred reactor closure: combustion model formulation and implementation details. *Appl Energy* 2018;225:637–55.
- [18] Chitgarha F, Mardani A. Assessment of steady and unsteady flamelet models for MILD combustion modeling. *Int J Hydrogen Energy* 2018;43:15551–63.
- [19] Farokhi M, Birouk M. Assessment of fractal/wrinkling theories for describing turbulent reacting fine structures under MILD combustion regimes. *Combust Sci Technol* 2020: 1–27 [in Press].
- [20] De A, Oldenhof E, Sathiah P, Roekaerts DJEM. Numerical simulation of Delft-Jet-in-Hot-Coflow (DJHC) flames using the EDC model for turbulence-chemistry interaction. *Flow Turb Combust* 2011;87:537–67.
- [21] De A, Dongre A. Assessment of turbulence-chemistry interaction models in MILD combustion regime. *Flow Turb Combust* 2015;94:439–78.
- [22] Labahn JW, Dovizio D, Devaud CB. Numerical simulation of the Delft-Jet-in-Hot-Coflow (DJHC) flame using Conditional Source-term Estimation. *Proc Combust Inst* 2015;35:3547–55.
- [23] Labahn JW, Devaud CB. Large Eddy Simulations (LES) including Conditional Source-term Estimation (CSE) applied to two Delft-Jet-in-Hot-Coflow (DJHC) flames. *Combust Flame* 2016;164:68–84.
- [24] Li Z, Lewandowski MT, Contino F, Parente A. Assessment of on-the-fly chemistry reduction and tabulation approaches for the simulation of moderate or intense low-oxygen dilution combustion. *Energy Fuels* 2018;32:10121–31.
- [25] Lewandowski MT, Ertesvåg IS. Analysis of the Eddy Dissipation Concept formulation for MILD combustion modelling. *Fuel* 2018;224:687–700.
- [26] Abtahizadeh E, de Goey P, van Oijen J. LES of Delft Jet-in-Hot Coflow burner to investigate the effect of preferential diffusion on autoignition of CH₄/H₂ flames. *Fuel* 2017;191:36–45.
- [27] Gran IR, Magnussen BF. A numerical study of a bluff-body stabilized diffusion flame. Part 2. Influence of combustion modeling and finite-rate chemistry. *Combust Sci Technol* 1996;119:191–217.
- [28] Farokhi M, Birouk M. A new EDC approach for modeling turbulence/chemistry interaction of the gas-phase of biomass combustion. *Fuel* 2018;220:420–36.
- [29] Evans MJ, Petre C, Medwell PR, Parente A. Generalisation of the eddy-dissipation concept for jet flames with low turbulence and low Damköhler number. *Proc Combust Inst* 2019;37:4497–505.
- [30] Oldenhof E, Tummers MJ, van Veen EH, Roekaerts DJEM. Conditional flow field statistics of jet-in-hot-coflow flames. *Combust Flame* 2013;160:1428–40.
- [31] Oldenhof E, Tummers MJ, van Veen EH, Roekaerts DJEM. Ignition kernel formation and lift-off behaviour of jet-in-hot-coflow flames. *Combust Flame* 2010;157:1167–78.
- [32] Magnussen BF. The Eddy Dissipation Concept: a bridge between science and technology. In *ECCOMAS Thematic Conference on Computational Combustion*, Lisbon, Portugal, 21–24 June, 2005.
- [33] Pope SB. An explanation of the turbulent round-jet/plane-jet anomaly. *AIAA J* 1978;16:279–81.
- [34] Or CM, Lam KM, Liu P. Potential core lengths of round jets in stagnant and moving environments. *J Hydro-Environ Res* 2011;5:81–91.
- [35] Nathan GJ, Mi J, Alwahabi ZT, Newbold GJR, Nobes DS. Impacts of a jet's exit flow pattern on mixing and combustion performance. *Prog Energy Combust Sci* 2007;32:496–538.
- [36] Lewandowski MT, Pluszka P, Pozorski J. Influence of inlet boundary conditions in computations of turbulent jet flames. *Int J Numer Methods Heat Fluid Flow* 2018;28:1433–56.
- [37] Lysenko DA, Ertesvåg IS, Rian KE. Numerical simulation of non-premixed turbulent combustion using the Eddy Dissipation Concept and comparing with the steady laminar flamelet model. *Flow Turb Combust* 2014;93:577–605.
- [38] Lewandowski MT, Pozorski J. Assessment of turbulence-chemistry interaction models in the computation of turbulent non-premixed flames. *J Phys: Conf Ser* 2016;760(012015):1–8.
- [39] Cavaliere A, de Joannon M. MILD combustion. *Prog Energy Combust Sci* 2004;30:329–66.
- [40] Weber R, Smart JP, vd Kamp W. On the (MILD) combustion of gaseous, liquid, and solid fuels in high temperature preheated air. *Proc Combust Inst* 30:2005;2623–2629.
- [41] Habibi A, Mercier B, Roekaerts D. Turbulence radiation interaction in Reynolds-averaged Navier-Stokes simulations of nonpremixed piloted turbulent laboratory-scale flames. *Combust Flame* 2007;151:303–20.
- [42] Chui EH, Raithby GD. Computation of radiant-heat transfer on a non-orthogonal mesh using the finite-volume method. *Numer Heat Transfer Part B* 1993;23:269–88.
- [43] Pitsch H. Unsteady flamelet modeling of differential diffusion in turbulent jet diffusion flames. *Combust Flame* 2000;123:358–74.
- [44] Barlow RS, Fiechtner GJ, Cartner CD, Chen JY. Experiments on the scalar structure of turbulent CO/H₂/N₂ jet flames. *Combust Flame* 2000;120:549–69.
- [45] Kim SK, Kim Y. Assessment of the eulerian particle flamelet model for nonpremixed turbulent jet flames. *Combust Flame* 2008;154:232–47.
- [46] Cuoci A, Frassoldati A, Buzzi Ferraris G, Faravelli T, Ranzi E. The ignition, combustion and flame structure of carbon monoxide/hydrogen mixtures. Note 2: Fluid dynamics and kinetic aspects of syngas combustion. *International Journal of Hydrogen Energy* 2007;32:3486–500.
- [47] Egoľopoulos FN, Hansen N, Ju Y, Kohse-Höinghaus K, Law CK, Qi F. Advances and challenges in laminar flame experiments and implications for combustion chemistry. *Prog Energy Combust Sci* 2014;43:36–67.
- [48] Kazakov A, Frenklach M. Reduced reaction set based on GRI-Mech 1.2: DRM19. <http://www.me.berkeley.edu/drm>. Accessed: 2015-08-15.
- [49] Bilger RW, Stårner SH, Kee RJ. On reduced mechanisms for methane-air combustion in nonpremixed flames. *Combust Flame* 1990;80:135–49.
- [50] Luan C, Xu S, Shi B, Tu Y, Liu H, Li P, Liu Z. Re-recognition of MILD combustion regime by initial conditions of Tin and XO₂ for methane in a non-adiabatic well-stirred reactor. *Energy Fuels* 2020:1–39 [in Press].
- [51] Pope SB. Computationally efficient implementation of combustion chemistry using in-situ adaptive tabulation. *Combust Theory Model* 1997;1:41–63.
- [52] Sabia P, de Joannon M, Picarelli A, Chinnici A, Ragucci R. Modeling negative temperature coefficient region in methane oxidation. *Fuel* 2012;91:238–45.
- [53] Lavadera ML, Sabia P, Sorrentino G, Ragucci R, de Joannon M. Experimental study of the effect of CO₂ on propane oxidation in a jet stirred flow reactor. *Fuel* 2016;184:876–88.
- [54] Tu Y, Yang W, Liu H. A refined global reaction mechanism for gently preheated MILD combustion of methane. *Energy Fuels* 2017;31:10144–57.
- [55] Mercier B, Dick E, Vierendeels J, De Langhe C. Determination of ϵ at inlet boundaries. *Int J Numer Methods Heat Fluid Flow* 2002;12:65–80.
- [56] Weller HG, Tabor G, Jasak H, Fureby C. A tensorial approach to computational continuum mechanics using object-oriented techniques. *Comput Phys* 1998;12(6):620–31.
- [57] Cuoci A, Frassoldati A, Faravelli T, Ranzi E. OpenSMOKE++: an object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms. *Comput Phys Commun* 2015;192:237–64.
- [58] Li Z, Malik MR, Cuoci A, Parente A. Edcsmoke: a new combustion solver for stiff-chemistry based on openFOAM. *Proc Int Conf Numer Anal Appl Math* 2017;1863:180004.
- [59] Chua LP, Antonia RA. Turbulent Prandtl number in a circular jet. *Int J Heat Mass Transfer* 1990;33:331–9.
- [60] Goldberg UC, Palaniswamy S, Batten P, Gupta V. Variable turbulent Schmidt and Prandtl number modeling. *Eng Appl Comput Fluid Mech* 2010;4:511–20.
- [61] Medwell PR, Kalt PAM, Dally BB. Imaging of diluted turbulent ethylene flames stabilized on a Jet in Hot Coflow (JHC) burner. *Combust Flame* 2008;152:100–13.