A numerical study of a cyclonic combustor under MILD conditions using non-adiabatic tabulated chemistry

Z. X. Chen,^{*,†} N. A. K. Doan,[†] X. J. Lv^{1,†}, N. Swaminathan,[†] G. Ceriello,[‡] G. Sorrentino,[‡] and A. Cavaliere[‡]

[†]*Department of Engineering, University of Cambridge, CB2 1PZ, UK*

[‡]*DICMAPI - University of Federico II of Naples, Piazzale Tecchio, 80, 80125 Naples, Italy*

E-mail: zc252@cam.ac.uk

Abstract

A cyclonic burner operating under moderate or intense low-oxygen dilution (MILD) conditions is simulated using a Perfectly Stirred Reactor (PSR) incorporated within a tabulated chemistry approach. A presumed joint probability density function (PDF) method is utilised with appropriate sub-models for the turbulence-chemistry interaction. Non-adiabatic effects are included in the PSR calculation to take into account the effects of non-negligible wall heat loss in the burner. Five different operating conditions are investigated and the computed mean temperatures agree well with measurements. A substantial improvement is observed when the non-adiabatic PSR is used highlighting the importance of heat transfer effects for burner configurations involving internal exhaust gas recirculation (EGR). Furthermore, enhanced reaction homogeneity is observed in this cyclonic configuration for the globally lean case, leading to a more spatially uniform temperature variation with MILD combustion.

¹On leave from Turbomachinery Institute, School of Mechanical Engineering, Shanghai Jiao Tong University. Shanghai 200240, China

1 Introduction

Currently, fossil fuel combustion is still the world's major energy source and will remain so in the foreseeable future. Due to the demand for even more efficient and less polluting combustion devices, alternative combustion concepts are constantly explored. Among these, Moderate or Intense Low-oxygen Dilution (MILD) combustion has been recognised as an attractive approach which can achieve both high thermal efficiency and low pollution simultaneously.¹⁻³ MILD combustion relies on the preheating and dilution of the reactant mixture which is obtained using exhaust gas recirculation. The recirculation can either be external⁴ or internal^{5,6} to the combustion chamber. Under these conditions, MILD combustion is then defined as occurring when the reactant temperature, T_r , is higher than its auto-ignition temperature, T_{ign} , and the temperature rise after combustion, $\Delta T = T_p - T_r$, is smaller than T_{ign} .³ As a result of these characteristics, the energy efficiency is improved by the use of exhaust gas while the emission is substantially reduced resulting from the homogeneous heat release with low peak of temperature.¹⁻³

In the past, the Jet in Hot Coflow (JHC) configuration has been studied both experimentally^{4,7-10} and numerically¹¹⁻¹⁶ as a representative of MILD combustion. Indeed, this simple configuration has allowed for precise laser measurements^{4,8} of various flow and thermochemical quantities providing physical insights into several key features of this combustion mode such as the importance of autoignition¹⁰ and the role of turbulence in promoting thicker reaction zones.¹⁷ However, other representative characteristics of MILD combustion commonly existing in practical burners with internal EGR are absent in the JHC configuration. For example, the homogeneous temperature field and mild gradient of species were observed in the original furnace-like experimental configurations with strong recirculation of burnt gases.^{2,5,18,19} These behaviours were also observed in the Direct Numerical Simulation (DNS)^{20,21} studies of MILD combustion with internal EGR showing additional physical complexities with an interplay among ignition, propagating and interacting reaction zones with premixed and non-premixed combustion attributes. The residence time, diluent composition

and the role of recirculation pattern were also found to be highly influential in establishing MILD combustion in these furnace-like burners.^{22–26}

In recent years, numerical simulations have become an essential tool in improving our understanding of the physical phenomena occurring in MILD combustion burners. However, most studies have focused on the study of the JHC using, for example, the Eddy Dissipation Concept (EDC) model,^{11,27} Conditional Moment Closure (CMC),¹³ transported probability density function (TPDF) approaches^{12,14} or models based on finite-rate chemistry closure.¹⁶ Indeed, these numerical efforts have substantially improved our understanding on modelling combustion under MILD conditions. However, most of these models treat the combustion chemistry in an explicit manner, i.e., all species considered in the chemical mechanism are calculated along with the turbulent flow, leading to high computational costs especially for industrial applications. The alternative modelling approach is to use tabulated chemistry and thus more economical computation is achieved by decoupling the chemistry and flow calculations. However, such approaches require a base chemistry solution which could be obtained from laminar flames,²⁸ igniting mixing layers,²⁹ zero-dimensional (0D) reactors, etc. Among these, the Perfectly Stirred Reactor (PSR) was shown to be a promising candidate in a validation study,¹⁵ providing the same level agreement with the JHC experiments as that by the sophisticated TPDF models with a gain of computational cost by an order of magnitude which is attractive for practical purposes.

In most tabulated chemistry applications, adiabatic conditions are assumed because in conventional systems, i.e., JHC, bluff-body or swirl stabilised, combustion typically occurs far from the burner walls and the mixture residence time is small compared to the heat conduction time scales. Several attempts^{30–34} have been made to investigate heat loss effects in those system showing only minor influences. However, for furnace-like MILD burners, the heat loss effects, e.g., conduction and radiation to the walls, are more influential because of the confinement and longer residence time due to internal EGR,^{26,35,36} posing great challenges for MILD combustion simulations. Therefore, further modelling consideration on the

heat loss effects is needed for tabulated chemistry approaches to be applied for more realistic experimental configurations and such attempts are seldom in the literature of MILD combustion. This requires a consistent treatment of heat loss not only in the turbulent flow simulation through energy transport but also in the base chemistry calculation where the thermo-chemical processes are influenced by the change of temperature.

Thus, the objective of this work is to fill this gap by simulating the cyclonic MILD combustor investigated experimentally by Sorrentino and coworkers^{23,29,35,37} using a non-adiabatic tabulated chemistry approach. This modelling framework is an extension of that proposed in Ref.¹⁵ by incorporating PSR calculations with a range of heat loss levels which adds another dimension represented by enthalpy to the chemistry tabulation. The simulation results are compared with the experimental data to assess the validity of this approach for different operating conditions. The heat loss effects are elucidated by comparing the results obtained using the adiabatic model. Furthermore, the MILD combustion features appearing in this cyclonic burner with internal EGR are studied and the effects of various operating parameters tested are explained on a physical basis.

This paper is organised as follows. A brief description of the modelling framework is provided in Section 2. Details on the experiment under study and the numerical setup are provided in Section 3. The results of the simulations are discussed in Section 4. Conclusions are summarised in the final section.

2 Modelling methodology

2.1 Governing equations

Three-dimensional Favre-averaged mass and momentum conservation equations are solved to account for the flow motions in the cyclonic burner with variable density due to combustion

heat release:³⁸

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{U}}) = 0, \quad (1)$$

$$\bar{\rho} \frac{D \tilde{\mathbf{U}}}{Dt} = -\nabla \bar{p} + \nabla \cdot \boldsymbol{\tau}_{\text{eff}}, \quad (2)$$

where $\bar{\rho}$ is the mean density of the local mixture, $\tilde{\mathbf{U}}$ is the Favre mean velocity vector and $\bar{p}$ is the mean thermodynamic pressure. The effective viscous tensor is the sum of the mean viscous and the Reynolds stresses: $\boldsymbol{\tau}_{\text{eff}} \equiv \bar{\boldsymbol{\tau}} - \bar{\rho} \widetilde{\mathbf{u}'' \mathbf{u}''} = \nabla \cdot \left[2(\bar{\mu} + \mu_t) \left(\tilde{\mathbf{S}} - (\nabla \cdot \tilde{\mathbf{U}}) \mathbf{I}/3 \right) \right]$, where $\bar{\mu}$ and μ_t are the laminar and turbulent dynamic viscosities respectively, with $\tilde{\mathbf{S}}$ and $\mathbf{I}$ being the mean rate-of-strain tensor and the identity matrix. The turbulent viscosity is modelled using the two-equation RNG (Re-Normalisation Group) $\tilde{k}$ - $\tilde{\varepsilon}$ approach^{29,39} for this study to capture complex turbulent flows in the cyclonic burner and a sensitivity study on the turbulence model is shown later in Section 4.

The turbulent mixing between the fuel and preheated oxidiser inside the burner is described by a mixture fraction, Z , using Bilger's formulation⁴⁰ and the modelled transport equations for the mean and variance solved in the simulation are written as

$$\bar{\rho} \frac{D \tilde{Z}}{Dt} = \nabla \cdot \left[\left(\bar{\mu} + \frac{\mu_t}{\text{Sc}_t} \right) \nabla \tilde{Z} \right], \quad (3)$$

$$\bar{\rho} \frac{D \widetilde{Z'^2}}{Dt} = \nabla \cdot \left[\left(\bar{\mu} + \frac{\mu_t}{\text{Sc}_t} \right) \nabla \widetilde{Z'^2} \right] + 2 \frac{\mu_t}{\text{Sc}_t} |\nabla \tilde{Z}|^2 - 2 \bar{\rho} \tilde{\chi}_Z, \quad (4)$$

where a turbulent Schmidt number of $\text{Sc}_t = 0.7$ is used to relate the turbulent diffusion processes of the scalar and velocity.¹⁵ The mean scalar dissipation rate is modelled using the linear-relaxation approximation: $\tilde{\chi}_Z \approx C_d \left(\tilde{\varepsilon} / \tilde{k} \right) \widetilde{Z'^2}$ with $C_d = 1.0$, following previous studies.^{41,42} A normalised progress variable, c , defined using the sum of CO and CO₂ mass fractions⁴¹ is used to describe the propane-air combustion progress for this study. The

Favre-averaged transport equations for c and its variance are:

$$\bar{\rho} \frac{D\tilde{c}}{Dt} = \nabla \cdot \left[\left(\bar{\mu} + \frac{\mu_t}{Sc_t} \right) \nabla \tilde{c} \right] + \overline{\dot{\omega}_c^-}, \quad (5)$$

$$\bar{\rho} \frac{D\widetilde{c'^2}}{Dt} = \nabla \cdot \left[\left(\bar{\mu} + \frac{\mu_t}{Sc_t} \right) \nabla \widetilde{c'^2} \right] + 2 \frac{\mu_t}{Sc_t} |\nabla \tilde{c}|^2 - 2 \bar{\rho} \tilde{\chi}_c + 2 \overline{c'' \dot{\omega}_c^-}, \quad (6)$$

where the scalar dissipation rate $\tilde{\chi}_c$ requires a more sophisticated closure for progress variable than that for mixture fraction and the model detailed in Ref.¹⁵ is adopted for this study. Note that here the mean reaction rate, $\overline{\dot{\omega}_c^-}$, includes the heat loss effects at the reactor (PSR) level and thus is denoted by the superscript, $-$, to distinguish from the adiabatic ones used in the earlier studies.^{15,29} The value of $\overline{\dot{\omega}_c^-}$ not only varies with the mean $\tilde{Z}$, $\tilde{c}$ and their variances, $\widetilde{Z'^2}$ and $\widetilde{c'^2}$ but also depends on the local total enthalpy of the mixture, h . Thus, the Favre-averaged transport equation for h ,

$$\bar{\rho} \frac{D\tilde{h}}{Dt} = \nabla \cdot \left[\left(\bar{\mu} + \frac{\mu_t}{Pr_t} \right) \nabla \tilde{h} \right], \quad (7)$$

is solved, where the turbulent Prandtl number is $Pr_t \approx 0.7$. As a initial attempt, gas-phase radiation is not considered for this study. However, the heat losses through the burner walls are considered and modelled using a wall heat flux:

$$\mathbf{q}_w = \mathcal{H}_w (T - T_w) \mathbf{n}, \quad (8)$$

with $\mathcal{H}_w$ and T_w , respectively being the material heat transfer coefficient and temperature of the burner walls, and $\mathbf{n}$ is the unit normal vector of the wall surface. The internal near-wall gas temperature, T , is taken as the temperature of the numerical cell next to the wall boundary, which is obtained using Eqs. (7) and (12). Note that $\mathbf{q}_w$ is included as a boundary condition at the combustor walls. The heat transfer coefficient is tuned in the simulations so that the computed near-wall fluid temperature matches the measured value.

The balance among the heat fluxes of gas-phase radiation, conduction through solid wall, and the convection and radiation on the outer surface of the wall, dictates the near-wall interior fluid temperature in reality. This complex balancing is modelled and captured using a simple expression in Eq. (8) and by tuning $\mathcal{H}_w$. Although this is a crude approximation for the combined effects, it serves the purpose here. Ideally, one would need to include all of these effects through explicit modelling of the conduction, radiation and convection processes, i.e., using conjugate heat transfer approaches. However, the above approximation is applied here as a first attempt to incorporate the heat loss effects into the widely used tabulated chemistry approach which is commonly assumed to be adiabatic. The implementation for this is non-trivial due to the decoupling between the chemistry and turbulent flow calculations, and the physical consistencies need to be kept carefully for the heat loss processes in these separated calculations.

2.2 PSR with heat loss

Figure 1 presents a schematic of the non-adiabatic PSR calculation performed using the chemical kinetics solver CANTERA.⁴³ The standard set of unsteady 0D PSR equations are

Fig. 1: Schematic of the non-adiabatic PSR.

solved and the heat loss sink term is included in the mixture enthalpy equation.⁴⁴ Depending on the temperature and composition of the fuel and oxidiser streams for a given operating condition, the initial state of the reactor is determined for different mixture fractions cov-

ering the entire reactive range. A constant residence time of $\tau = 0.5$ s estimated in the experiments²⁴ is used for all PSR simulations. To account for the heat loss, a heat flux is specified in a similar manner as in Eq. (8) and an ambient temperature of 1045 K is given for the surrounding environment. This value is the measured temperature at the outer wall and thus is a good estimate for the far-field temperature of the heat reservoir. For a given mixture fraction, PSR calculations are performed for different values of $\mathcal{H}_w$ to allow for a range of heat loss levels. The maximum value of $\mathcal{H}_w$ is determined such that the final state temperature approaches the ambient temperature at the end of residence time.

Figure 2 shows temporal variations of temperature and heat release rate for the stoichiometric propane-air mixture of experimental case CS-1 (see Table 2) in a PSR for three heat loss levels denoted by different heat transfer coefficients, $\mathcal{H}_w$. The adiabatic case ($\mathcal{H}_w = 0$)

Fig. 2: Temporal variation of temperature (top) and heat release rate (bottom) in the PSR for four typical heat loss levels.

is also shown for comparison. It is seen that as the heat loss increases the temperature drops drastically after ignition. However, the final temperature does not always reach the ambient temperature of 1045 K due to the insufficient residence time even for the value of $\mathcal{H}_w = 3000$ W/m²/K, which is two orders of magnitude higher than the measured value of 41.84 for the burner walls. This is consistent with the experiments where the overall residence time of the mixture inside the burner is typically smaller than the wall cooling time suggesting that chemical reactions may not be largely influenced by the heat loss for highly

reactive mixtures. It is noticeable in Fig. 2 that the ignition is faster for the non-adiabatic cases because the initial reactant temperature is lower than the heat reservoir temperature, i.e., $T < T_w$ in Eq. 8, and hence the PSR is heated by the environment during the early stages. However, the magnitude of heat release rate is almost the same since the time-scales of chemical reactions are much smaller than that for the heat exchange process. This can be further seen in Fig. 3 showing the major (C_3H_8 and CO_2) and pollutant (CO and NO) species variations in the PSR with different heat loss levels. Following the temperature vari-

Fig. 3: Typical species mass fraction variation of C_3H_8 , CO_2 , CO and NO in the PSR for four typical heat loss levels (see legend in Fig. 2).

ations shown earlier, the reactions take place earlier for high heat loss cases (lower h) due to the ambient heat effect and the overall evolution remains rather similar for all four representative species presented despite the drastic temperature drop after ignition. This is quite different from the previous studies on non-adiabatic flamelets, in which flame quenching was

observed after the heat loss reached a certain level.^{30,32} The reason is that the peak temperature is much higher, up to 2200 K for stoichiometric hydrocarbon-air flames, leading to large temperature gradient and hence more severe heat losses. In contrast, the PSR simulated here with MILD conditions has a peak around 1550 K and the chemical reactions are less influenced by the heat loss.

For each experimental case simulated, 200 (in Z) $\times$ 10 (in h) PSR calculations are performed. Using these two control variables along with the progress variable, all the PSR quantities can be mapped into a three-dimensional manifold and the reaction rate, $\dot{\omega}_c^-(Z, h, c)$, is then used to model the source terms in Eqs. (5) and (6):

$$\overline{\dot{\omega}_c^-} = \int \int \int \dot{\omega}_c^-(\xi, \eta, \zeta) P(\xi, \eta, \zeta) d\xi d\eta d\zeta, \quad (9)$$

$$\overline{c''\dot{\omega}_c^-} = \int \int \int (\zeta - \tilde{\zeta}) \dot{\omega}_c^-(\xi, \eta, \zeta) P(\xi, \eta, \zeta) d\xi d\eta d\zeta, \quad (10)$$

where ξ , η and ζ are the sample space variables for Z , h and c respectively. The joint probability density function, $P(\xi, \eta, \zeta)$, signifies the statistical variations of the three control variables in the turbulent flow and it is modelled as

$$P(\xi, \eta, \zeta) = \beta(\xi; \tilde{Z}, \widetilde{Z'^2}) \times \delta(\eta - \tilde{h}) \times \beta(\zeta; \tilde{c}, \widetilde{c'^2}), \quad (11)$$

where the β -function is used for Z and c as in Refs.^{15,41} and a Dirac δ -function is adopted for h as a first attempt. Other thermo-chemical quantities such as the mixture effective specific heat capacity,⁴¹ $\tilde{C}_p^e$, and enthalpy of formation, $\tilde{h}_f^0$, are modelled in a similar manner as in Eq. (9). The temperature is determined using

$$\tilde{T} = \frac{\tilde{h} - \tilde{h}_f^0}{\tilde{C}_p^e} + T_0, \quad (12)$$

and $T_0 = 298.15$ K. The mixture effective specific heat capacity is temperature dependent

as demonstrated and discussed in previous studies.^{41,42} Here the mixture enthalpy (chemical+sensible) is transported using Eq. (7) whereas $\tilde{C}_p^e$ and $\tilde{h}_f^0$ are obtained using a presumed joint PDF approach which utilises the PSR calculation. Thus, the effect of wall heat conduction needs to be considered in both approaches and this allows us to study their individual effect on the temperature field by including one at a time. Depending on whether the heat flux is included in the PSR or for the $\tilde{h}$ equation (through its boundary condition), three models are established as listed in Table 1: Model-1 implies adiabatic burner with adiabatic PSR, Model-2 implies non-adiabatic with adiabatic PSR and Model-3 implies both burner and PSR are non-adiabatic.

Table 1: Model combination detail.

Model	1	2	3
Heat flux for $\tilde{h}$	No	Yes	Yes
Heat flux for PSR	No	No	Yes

3 Experimental and numerical details

3.1 Test case experiments

The experimental configuration of Sorrentino et al.²³ is studied here to investigate the MILD combustion of propane with diluted and preheated air. Experimental measurements on this burner have been reported in various previous studies^{23,29,35} and are compared here to numerical simulations. Propane was chosen as the reference fuel because it is an important fuel for several practical applications. Moreover, the propane/oxygen chemical kinetics is fundamentally important for all combustion processes of hydrocarbons, and it is well known and sufficiently simple. The elementary reactions of propane combustion and its intermediate oxidation species are a central part of the mechanisms which describe the combustion of any hydrocarbon or oxygenated fuel. Also, propane can partially represent the thermochemical

and combustion properties of larger hydrocarbons.

Figure 4 shows a sketch of the mid-plane section of this laboratory-scale burner ($0.2 \times 0.2 \times 0.05 \text{ m}^3$) alongside a photograph of the burner. The combustor is built using heat-insulating material and is located within an electrically heated ceramic oven to minimize the heat losses. Two oxidiser and fuel jets are positioned at opposite corners of the combustion chamber to produce a cyclonic flow field while the outlet is located at the centre of the top plane, see Fig. 4. The oxidiser and fuel jets are respectively placed at 2 cm and 4.5 cm from the side wall. The fuel jets have diameter of 0.08 cm and C_3H_8 diluted with N_2 is injected at 50 m/s at ambient temperature (300 K) while the oxidiser jets have a diameter of 0.8 cm and O_2 diluted with N_2 is injected at 38m/s at a preheated temperature T_{ox} . Experiments were performed to operate the combustor in a non-premixed mode. Therefore, the main pre-heated flow is composed by oxygen and diluent (N_2) and the fuel flow (propane) is injected with N_2 . The fuel jet is partially diluted with N_2 to keep its velocity independent of the carbon/oxygen feed ratio. This combination of high recirculation through the cyclonic configuration with preheated oxidiser and diluted fuel allows for the stable operation of MILD combustion in this burner operated at atmospheric pressure.

Temperature was measured using two sliding thermocouples (type N, Nisil - NiCroSil) with a diameter of 1.5 mm located in the mid- y plane of the burner with an accuracy of $\pm 2.2 \text{ K}$. These thermocouples were then placed in alumina tube of 2 mm of diameter to minimize their effects on the flow pattern. The central and lateral thermocouples are placed as depicted in Fig. 4. The uncertainties in the measurements are linked to convective and radiation effects. The convective effects are important close to the oxidiser inlet and radiative effects are non-negligible close to the walls. These uncertainties in the lateral measurements are $\pm 2\%$ and $\pm 6\%$ respectively for the convection and radiation, and $\pm 1\%$ and $\pm 1.5\%$ for the central measurements. These uncertainties on the thermocouples measurements were estimated by considering a heat balance between the thermocouples and the flow through forced convection and radiative heat exchange between the thermocouple and the wall. The

Fig. 4: Sketch of the mid-plane section of the cyclonic burner.²³

overall heat transfer coefficient of the reactor was calculated to be $41.84 \text{ W/m}^2/\text{K}$ using the thermal resistances in series concept based on the system boundary conditions, namely, the oven temperature in which the cyclonic chamber is located and the inlet flow temperature and velocity, considering a non-reactive case. Such value was also confirmed by an overall heat balance on the system by measuring the gas temperature at the exit. The uncertainty related to the heat exchange coefficient value was evaluated as about 8% on the basis of flow rate and temperature measurement accuracies.

Five different experimental conditions described in Table 2 are studied here. These have already been partially reported in previous studies.^{23,35} The effects of T_{ox} and equivalence ratio, Φ , are investigated. In all cases, the mean residence time τ is kept constant at 0.5 s and the global inlet content of N_2 is fixed at 94 % in volume. The equivalence ratio is changed by modifying the fuel and oxidiser compositions as reported in Table 2. Three different oxidiser temperatures, T_{ox} , are also considered.

Table 2: Details of experimental cases under study.

Case	ϕ	T_{ox}	Fuel	Oxidiser	P_{th} [kW]
		[K]	$X_{\text{C}_3\text{H}_8} / X_{\text{N}_2}$	$X_{\text{O}_2} / X_{\text{N}_2}$	
CL-1	0.33	1045	0.0856 / 0.914	0.059 / 0.941	0.36
CS-1	1	1045	0.23 / 0.77	0.052 / 0.948	0.97
CR-1	1.67	1045	0.343 / 0.657	0.047 / 0.953	1.45
CS-2	1	1075	0.222 / 0.778	0.053 / 0.947	0.94
CS-3	1	1125	0.212 / 0.788	0.053 / 0.948	0.89

3.2 Numerical setup

The computational domain includes the fuel and oxidiser inlet tubes, combustion chamber and the outlet duct. This domain is discretised using an unstructured numerical grid comprising 596,000 hexahedral cells as shown in Fig. 5a. Mesh refinement is applied in the inlet

Fig. 5: (a) Volume view of the numerical grid (b) Iso-surfaces of vorticity magnitude (red) threshold at 20% of its maximum and of enthalpy threshold at 50% (green) and 75% (blue) of its maximum.

region of the jets to have a good resolution for the shear layer because of the strong turbulence in this region as can be seen in Fig. 5b by a vorticity iso-surface (red coloured). The cyclonic motion of the flow also generates turbulence forming a vortex core in the centre of the burner (the central cylinder in Fig. 5b). This strong swirling motion recirculates the hot products (indicated by high-enthalpy iso-surfaces) inside the cyclonic burner, which is illustrated by the green toroidal iso-surface cycling around. As a result of this internal EGR, MILD combustion is established with a homogeneous temperature field and a progressive

increase in temperature as will be discussed in Section 4.

The commercial software ANSYS Fluent 18.1 is used as the flow solver for this work. The built-in energy transport and combustion models are disabled and instead the framework described in Section 2 is implemented using User Defined Scalars and Memories (UDS and UDM).⁴² The detailed chemical mechanism POLIMI C1-C3⁴⁵ is used for propane-air combustion in this study. For the inlet boundaries, top-hat velocity profiles are given for both fuel and oxidiser streams. The no-slip condition is employed for all the walls and pressure outlet is specified for the exhaust exit. The mixture fraction value is specified to be 1 and 0 for the fuel and oxidiser streams respectively. For the progress variable, 0 is specified for both streams. The inlet enthalpies are determined based on the thermodynamic properties of the inflow which vary for different cases. All scalar gradients are set to be zero for the walls except enthalpy, for which a heat flux is specified using Eq. (8). The control variables, $\tilde{Z}$, $\tilde{Z}''^2$, $\tilde{h}$, $\tilde{c}$ and $\tilde{c}''^2$, are solved as UDS using their transport equations. The various sources and sinks for these equations are tabulated in a five-dimensional ($72 \times 15 \times 10 \times 31 \times 21$) lookup table using an in-house integration code incorporated with CANTERA prior to the Fluent simulations. For each case in Table 2, a different lookup table is generated because of the difference in composition of the fuel and oxidiser streams. The table generation time is about 1 hour on the ARCHER Supercomputer using 72 cores. A fully converged reacting flow solution takes about 1.5 hours on a 20-core Dell Workstation.

4 Results – model validation and discussion

To visualise the general combustion behaviours inside the cyclonic burner, Fig. 6 shows the half mid-plane contours of mean reaction rate and temperature for the CS-1 case computed using the Model 3 (see Table 1). It is seen that the temperature distribution is quite homogeneous inside the burner as one would expect for MILD combustion. Due to the strong cyclonic motion of the burnt gases (indicated by the white arrow), the fuel jet is pushed

Fig. 6: Mid- z -plane contours of reaction rate (top) and temperature (bottom).

towards the oxidiser jet and merges with it a few diameters downstream of the oxidiser jet exit. This indicates a fast mixing pattern and because the fuel is already heated by the burnt gas before mixing with the oxidiser, the resulting mixture reactivity is quite high and thus the reactions occur quickly after mixing as suggested by the short length of the reaction zone shown in Fig. 6. The reaction zone lies in the shear layer of the oxidiser jet suggesting that in MILD combustion reaction is mainly controlled by the oxidiser, not fuel which dictates the reaction zone location in conventional diffusion flames. A circular low-temperature zone is present in the centre of the burner as seen in Fig. 6 and this was also observed in the experiments, resulting from the strong heat loss close to the outlet. It is worth remarking here that the fuel-to-oxidiser ratio of the bulk mass flow rates is very small, i.e., $\rho_f U_f A_f / \rho_{ox} U_{ox} A_{ox} < 1/100$ with A being the cross-sectional area of the inflow pipes and thus the low temperature fuel jet is unable to penetrate into the oxidiser jet although there is a strong momentum in the transverse direction. As a result, the measured temperature along the oxidiser jet centreline is always larger than the inlet value T_{ox} and this is important for the model validation as one shall see later in this section.

Considering the complex turbulent flow inside this cyclonic burner, it is worthwhile to examine the sensitivity of the numerical results to the turbulence model. Thus, three com-

monly used turbulence models are tested: the two-equation standard $k-\epsilon$ model, the RNG modification, and the Reynolds Stress Model (RSM). Fig. 7 compares the computed temperature profiles using these models with the experimental thermocouple measurements at the central and lateral positions (see Fig. 4). It can be seen that the simulation results given

Fig. 7: Sensitivity of temperature predictions to the turbulence model. Symbols are measurements with associated uncertainty, lines are computations.

by all three models agree well with the experimental data at the central position showing only minor differences. For the lateral position, the RSM model tends to overestimate the ignition along the measured line and the temperature starts to increase at about $x = 0.04$ m compared to that of $x = 0.025$ m for the $k-\epsilon$ and RNG models. In the experiments, however, the temperature rise was observed at even earlier position at $x = 0.01$ m, which is 1.2 diameter of the oxidiser jet downstream of the exit. It is well-known that the jet potential core sustains for few diameters on the centreline after the exit and the mixture composition remains the same, i.e., pure oxidiser in the present case. This means that at this position ($x = 0.01$ m), without mixing with the fuel stream, the mixture is still inflammable and hence ignition is unlikely to occur. It can be proven in Fig. 8 that the mixture fraction value is below the lean flammability limit (determined using PSR) for all three turbulence models used. Thus, the early temperature rise observed in the experiments is unlikely to be a mean flow behaviour but a consequence of some transient mixing effects. It is speculated that the high turbulent swirling flow enhances the mixing by pushing the fuel jet towards

Fig. 8: Mixture fraction variation along the lateral measuring line computed using three different turbulence models.

the oxidiser jet (see Fig. 6) and during this process the fuel jet occasionally breaks down into small pockets. Some of these fuel pockets penetrate into the oxidiser jet and then burn inside producing high local temperature. Another possibility can result from the limitation of thermocouple measurements as indicated by the relatively larger error bars for upstream locations. Nevertheless, the temperature variation inside the combustion chamber is predicted reasonably well for both the central and lateral positions, and the best-performing RNG turbulence model is adopted for the following discussions on the heat loss effects.

Figure 9 compares the measured²⁹ and computed temperatures along the central and lateral lines for cases CL-1, CS-1, CR-1 listed in Table 2. The numerical results (lines) shown are obtained from the simulations performed in the present study using models 1, 2 and 3 (see Table 1), and also from the previous study by Sorrentino et al.²⁹ using the built-in FGM model in ANSYS Fluent. It is worth remarking here that this FGM model utilised an adiabatic igniting mixing layer (IML)⁴⁶ as the canonical model to build the lookup table. The heat loss was considered only in the turbulent simulations through a thermal boundary condition for the burner walls as in Model-2 using the same heat transfer coefficient. It can be seen in Fig. 9 that all the models are able to reproduce the nearly constant temperature profile measured along the central line with a small dip in the middle. The purely adiabatic Model-1 over-predicts the temperature significantly indicating that the wall heat loss is

Fig. 9: Temperature variation along the central (left column) and lateral (right column) locations for cases CL-1 (top row), CS-1 (middle) and CR-1 (bottom). Symbols are measurements with associated uncertainty, lines are computations.

substantial at the global level and thus should be taken into account through the energy (enthalpy) transport equation. For the case CS-1, Fluent-FGM and Model-2 yield similar results as one would expect, both slightly under-predicting the central line temperature. By contrast, Model-3 captures the variation quite well for all three cases suggesting that the heat loss tends to be over-estimated when only considering the non-adiabatic effects in the Fluent simulations but not in the canonical configuration used to build the lookup table.

For the lateral line, however, Model-2 and Fluent-FGM largely under-predict the temperature for $x < 0.05$ m with an unphysical drop at the beginning (close to the oxidiser jet exit). It is remarked here that this unphysical behaviour may arise due to the inconsistency between the transported non-adiabatic $\tilde{h}$ and the tabulated adiabatic $\widetilde{C}_p^e$. As can be seen

in Fig. 9, Model-3 with the non-adiabatic PSR shows the correct behaviour for $x < 0.05$ m and the overall agreement with the measurement is improved substantially from the Model-2 and Fluent-FGM. For locations $x < 0.02$ m, where ignition already occurs in all three cases, no temperature rise is predicted in the simulation suggesting a strong penetration of the oxidiser jet. This has been noted earlier in Fig. 7b and the experimental uncertainty in this region was reported to be significantly larger compared to the downstream ($x > 0.1$ m). It is also worth remarking that the thermocouple had a non-negligible diameter of 2 mm compared to 8 mm for the oxidiser jet. Thus, the physical presence of the thermocouple could disturb the flow and act as a “flame holder” to stabilise reactions leading to higher temperature. It would be helpful to compare with laser-based temperature measurements with the flow/mixing field unaffected and this would be of interest for future studies. Nonetheless, the temperature distribution and its variation with Φ are predicted quite well by the Model-3 with a substantial improvement over the Fluent default FGM model.

Fig. 10: Temperature variation along the central (left column) and lateral (right column) locations for cases CS-2 (top row) and CS-3 (bottom row). Symbols are experimental measurements with associated uncertainty and lines are computations.

To further assess the performance of the models, temperature comparison is shown for

CS-2 and CS-3 cases with $T_{\text{ox}} = 1075$ and 1125 K respectively. The fully adiabatic Model-1 over-predicts the burnt temperature even more because the final-state temperature is higher than that in the $T_{\text{ox}} = 1045$ K cases leading to higher global heat loss. For the Model-3 with non-adiabatic effects considered at both the global and PSR levels, the comparisons similar to those discussed in Fig. 9 are observed showing an improved agreement with the experimental measurements.

To investigate the MILD combustion characteristics under different operating conditions, Fig. 11 depicts the reaction rate contours in the half mid-plane for the five cases listed in Table 2. Model-3 is used for these simulations. A considerable variation of reaction zone

Fig. 11: Reaction zone behaviour under different MILD conditions.

behaviour can be observed among these cases with varying global equivalence ratio (Φ) and oxidiser preheat temperature (T_{ox}). For the T_{ox} (1045 K) cases, the reaction zone behaviours between the stoichiometric and rich cases CS-1 and CR-1 are similar, i.e., it is located in the shear layer of the oxidiser jet and the peak value is about $20 \text{ kg/m}^3/\text{s}$. When T_{ox} increases

in CS-2 and CS-3, the peak reaction rate also increases as one would expect but the reaction zone shape and location remain almost the same as in CS-1.

In contrast, the lean case CL-1 shown in Fig. 11 is rather different. The peak reaction rate is much lower, about $10 \text{ kg/m}^3/\text{s}$, and it appears in the mixing layer between the fuel and oxidiser jets. In addition to the reaction zone in the shear layer of oxidiser jet, substantial reaction is also found around the fuel jet forming another reaction zone (marked using red box). This difference stems from the excess oxygen in the lean case and a large part of this oxygen is carried by the burnt gases recirculating inside the combustor as shown in Fig. 12. As discussed earlier in Fig. 6, the fuel jet is distorted by the swirling flow of burnt gases in

Fig. 12: Half mid-plane contours of oxygen mass fraction for the $T_{\text{ox}} = 1045 \text{ K}$ cases with different global equivalence ratios.

the transverse direction as soon as it enters the combustion chamber and with the oxygen content this forms an interesting configuration similar to jet-in-cross-flow. This distorted fuel jet behaviour can also result from the so-called “strong-jet/weak-jet” problem⁴⁷ where the weak jet entrains the strong jet following a parabolic arc trajectory as seen in Fig. 11 for case CL-1. As a result, the fuel jet has partially reacted before merging with the main stream of oxidiser, resulting in a more distributed reaction zone behaviour and lower NO_x production.

To further demonstrate this, Fig. 13 shows the conditional average of the mean reaction

rate on the mixture fraction for the five operating conditions studied. It is very clear that

Fig. 13: Conditional averages of the mean reaction rate on the mixture fraction.

the reaction in the lean case CL-1 spreads over a large range of mixture fraction up to 0.2 with no evident peaks. For the other four cases, however, a strong peak is found at around $Z = 0.02$ and the reaction rate becomes zero in the rich mixtures with $Z > 0.07$. This suggests that the cyclonic configuration operating under overall lean condition is promising for characterising MILD combustion and reach the distributed reaction zone regime observed in previous DNS studies.^{21,48} The jet-in-cross-flow and strong-jet/weak-jet mechanisms intrinsically established in this cyclonic combustor^{23,24} are helpful to achieve this, which is absent in other MILD combustion configurations such as the jet-in-hot-coflow^{4,8} and confined burners with inlet/outlets on the same plane.^{36,49} The distributed reactions lead to milder scalar gradient and temperature distribution,⁵⁰ which is desirable in practical applications for NO_x reduction.

5 Conclusions

A novel laboratory-scale cyclonic MILD combustion burner with internal Exhaust Gas Recirculation (EGR) is studied numerically using a non-adiabatic tabulated chemistry approach. The effect of heat transfer is included at the base chemistry level using Perfectly Stirred Reactor (PSR) and the mixture enthalpy is used as an additional control variable for the thermo-chemistry tabulation. Typical attributes of MILD combustion such as homogeneous temperature field and widely distributed reaction zones are captured well by the simulations. It is found that the wall heat loss is quite substantial in this burner and the temperature is predicted well only when the non-adiabatic effects are considered at both the global and PSR levels. An overall good agreement is obtained between the computed and measured temperature along two cross-burner measuring lines for five different MILD operating conditions. The results suggest that heat loss effects play an important role in such furnace-like burners and it needs to be included carefully at various, flow fields and reaction rate, modelling levels. Moreover, visualisation and conditional analysis of the mean reaction rate show a more distributed reaction zone behaviour in the overall lean equivalence ratio case. The cyclonic swirling motion of the burnt gases with excess air content gives rise to a favourable situation similar to the jet-in-cross-flow, and the strong-jet/weak-jet interaction also leads to enhanced mixing prior to combustion. Further experimental and numerical investigations could be devoted to better understand these mechanisms and their role in establishing MILD combustion in future studies.

Acknowledgement

ZXC and NS acknowledge the support of Mitsubishi Heavy industries, Japan. NAKD acknowledges the support of the Qualcomm European Research Studentship Fund. This work used the ARCHER UK National Supercomputing Service (<http://www.archer.ac.uk>) using computing time provided by the UKCTRF (e305). XJL acknowledges Shanghai Sailing

Talent Fellowship (No. 17YF1409800). GC, GS and AC greatly acknowledge the COST Action SMARTCATs (CM1404), supported by COST (European Cooperation in Science and Technology, <http://www.cost.eu>).

References

- (1) Wüning, J. A.; Wüning, J. G. Flameless oxidation to reduce thermal no-formation. *Prog. Energy Combust. Sci.* **1997**, *23*, 81–94.
- (2) Katsuki, M.; Hasegawa, T. The science and technology of combustion in highly preheated air. *Symp. Combust.* **1998**, *27*, 3135–3146.
- (3) Cavaliere, A.; de Joannon, M. Mild Combustion. *Prog. Energy Combust. Sci.* **2004**, *30*, 329–366.
- (4) Dally, B. B.; Karpetis, A. N.; Barlow, R. S. Structure of turbulent non-premixed jet flames in a diluted hot coflow. *Proc. Combust. Inst.* **2002**, *29*, 1147–1154.
- (5) Plessing, T.; Peters, N.; Wüning, J. G. Laseroptical investigation of highly preheated combustion with strong exhaust gas recirculation. *Symp. Combust.* **1998**, *27*, 3197–3204.
- (6) Krishnamurthy, N.; Paul, P. J.; Blasiak, W. Studies on low-intensity oxy-fuel burner. *Proc. Combust. Inst.* **2009**, *32*, 3139–3146.
- (7) Dally, B. B.; Riesmeier, E.; Peters, N. Effect of fuel mixture on moderate and intense low oxygen dilution combustion. *Combust. Flame* **2004**, *137*, 418–431.
- (8) Oldenhof, E.; Tummers, M. J.; van Veen, E. H.; Roekaerts, D. J. E. M. Ignition kernel formation and lift-off behaviour of jet-in-hot-coflow flames. *Combust. Flame* **2010**, *157*, 1167–1178.

- (9) Oldenhof, E.; Tummers, M. J.; van Veen, E. H.; Roekaerts, D. J. E. M. Conditional flow field statistics of jet-in-hot-coflow flames. *Combust. Flame* **2013**, *160*, 1428–1440.
- (10) Medwell, P. R.; Kalt, P. A. M.; Dally, B. B. Simultaneous imaging of OH, formaldehyde, and temperature of turbulent nonpremixed jet flames in a heated and diluted coflow. *Combust. Flame* **2007**, *148*, 48–61.
- (11) Christo, F.; Dally, B. B. Modeling turbulent reacting jets issuing into a hot and diluted coflow. *Combust. Flame* **2005**, *142*, 117–129.
- (12) 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*, 1464–1476.
- (13) Kim, S. H.; Huh, K. Y.; Dally, B. B. Conditional moment closure modeling of turbulent nonpremixed combustion in diluted hot coflow. *Proc. Combust. Inst.* **2005**, *30 I*, 751–757.
- (14) De, A.; Dongre, A. Assessment of Turbulence-Chemistry Interaction Models in MILD Combustion Regime. *Flow, Turbul. Combust.* **2015**, *94*, 439–478.
- (15) Chen, Z.; Reddy, V. M.; Ruan, S.; Doan, N. A. K.; Roberts, W. L.; Swaminathan, N. Simulation of MILD combustion using Perfectly Stirred Reactor model. *Proc. Combust. Inst.* **2017**, *36*, 4279–4286.
- (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*, 555–570.
- (17) Duwig, C.; Li, B.; Li, Z.; Aldén, M. High resolution imaging of flameless and distributed turbulent combustion. *Combust. Flame* **2012**, *159*, 306–316.

- (18) de Joannon, M.; Saponaro, A.; Cavaliere, A. Zero-dimensional analysis of diluted oxidation of methane in rich conditions. *Proc. Combust. Inst.* **2000**, *28*, 1639–1646.
- (19) Ozdemir, I. B.; Peters, N. Characteristics of the reaction zone in a combustor operating at mild combustion. *Exp. Fluids* **2001**, *30*, 683–695.
- (20) Minamoto, Y.; Swaminathan, N. Subgrid scale modelling for MILD combustion. *Proc. Combust. Inst.* **2015**, *35*, 3529–3536.
- (21) Doan, N. A. K.; Swaminathan, N.; Minamoto, Y. DNS of MILD combustion with mixture fraction variations. *Combust. Flame* **2018**, *189*, 173–189.
- (22) Szego, G.; Dally, B. B.; Nathan, G. Scaling of NO_x emissions from a laboratory-scale mild combustion furnace. *Combust. Flame* **2008**, *154*, 281–295.
- (23) Sorrentino, G.; Sabia, P.; de Joannon, M.; Cavaliere, A.; Ragucci, R. The Effect of Diluent on the Sustainability of MILD Combustion in a Cyclonic Burner. *Flow, Turbul. Combust.* **2016**, *96*, 449–468.
- (24) Sorrentino, G.; Sabia, P.; Bozza, P.; Ragucci, R.; de Joannon, M. Impact of external operating parameters on the performance of a cyclonic burner with high level of internal recirculation under MILD combustion conditions. *Energy* **2017**, *137*, 1167–1174.
- (25) Veríssimo, A. S.; Rocha, A. M. A.; Coelho, P. J.; Costa, M. Experimental and Numerical Investigation of the Influence of the Air Preheating Temperature on the Performance of a Small-Scale Mild Combustor. *Combust. Sci. Technol.* **2015**, *2202*, 150611114133006.
- (26) Li, P.; Wang, F.; Mi, J.; Dally, B. B.; Mei, Z. MILD Combustion under Different Premixing Patterns and Characteristics of the Reaction Regime. *Energy & Fuels* **2014**, *28*, 2211–2226.
- (27) 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, Turbul. Combust.* **2012**, *88*, 597–623.
- (28) Ihme, M.; See, Y. C. LES flamelet modeling of a three-stream MILD combustor: Analysis of flame sensitivity to scalar inflow conditions. *Proc. Combust. Inst.* **2011**, *33*, 1309–1317.
- (29) Sorrentino, G.; Göktolga, U.; de Joannon, M.; van Oijen, J. A.; Cavaliere, A.; de Goey, P. An experimental and numerical study of MILD combustion in a Cyclonic burner. *Energy Procedia* **2017**, *120*, 649–656.
- (30) Fiorina, B.; Baron, R.; Gicquel, O.; Thevenin, D.; Carpentier, S.; Darabiha, N. Modelling non-adiabatic partially premixed flames using flame-prolongation of ILDM. *Combust. Theory Model.* **2003**, *7*, 449–470.
- (31) Fiorina, B.; Veynante, D.; Candel, S. M. Modeling Combustion Chemistry in Large Eddy Simulation of Turbulent Flames. *Flow, Turbul. Combust.* **2014**, 3–42.
- (32) Cecere, D.; Giacomazzi, E.; Picchia, F. R.; Arcidiacono, N.; Donato, F.; Verzicco, R. A non-adiabatic flamelet progress-variable approach for les of turbulent premixed flames. *Flow, Turbul. Combust.* **2011**, *86*, 667–688.
- (33) Donini, A.; Bastiaans, R. J.; van Oijen, J. A.; de Goey, L. P. A 5-D Implementation of FGM for the Large Eddy Simulation of a Stratified Swirled Flame with Heat Loss in a Gas Turbine Combustor. *Flow, Turbulence and Combustion* **2017**, *98*, 887–922.
- (34) Lamouroux, J.; Ihme, M.; Fiorina, B.; Gicquel, O. Tabulated chemistry approach for diluted combustion regimes with internal recirculation and heat losses. *Combust. Flame* **2014**, *161*, 2120–2136.

- (35) De Joannon, M.; Sabia, P.; Sorrentino, G.; Bozza, P.; Ragucci, R. Small size burner combustion stabilization by means of strong cyclonic recirculation. *Proc. Combust. Inst.* **2017**, *36*, 3361–3369.
- (36) Li, P.; Dally, B. B.; Mi, J.; Wang, F. MILD oxy-combustion of gaseous fuels in a laboratory-scale furnace. *Combustion and Flame* **2013**, *160*, 933–946.
- (37) Sorrentino, G.; Sabia, P.; Bozza, P.; Ragucci, R.; De Joannon, M. Impact of external operating parameters on the performance of a cyclonic burner with high level of internal recirculation under MILD combustion conditions. *Energy* **2017**, *137*, 1167–1174.
- (38) Poinso, T.; Veynante, D. *Theoretical and Numerical Combustion*, 3rd ed.; Aquaprint, 2011; p 603.
- (39) Yakhot, V.; Orszag, S. A.; Thangam, S.; Gatski, T. B.; Speziale, C. G. Development of turbulence models for shear flows by a double expansion technique. *Phys. Fluids* **1992**, *4*, 1510–1520.
- (40) Bilger, R. W. Effects of Kinetics and Mixing in Turbulent Combustion. *Combust. Sci. Technol.* **1979**, *19*, 89–93.
- (41) Chen, Z.; Ruan, S.; Swaminathan, N. Simulation of turbulent lifted methane jet flames: Effects of air-dilution and transient flame propagation. *Combust. Flame* **2015**, *162*, 703–716.
- (42) Ruan, S.; Swaminathan, N.; Darbyshire, O. Modelling of turbulent lifted jet flames using flamelets: a priori assessment and a posteriori validation. *Combust. Theory Model.* **2014**, *18*, 295–329.
- (43) Goodwin, D. G.; Moffat, H. K.; Speth, R. L. Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes. 2017; Version 2.3.0.

- (44) <http://www.cantera.org/docs/sphinx/html/reactors.html>.
- (45) Ranzi, E.; Frassoldati, A.; Grana, R.; Cuoci, A.; Faravelli, T.; Kelley, A. P.; Law, C. K. Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels. *Prog. Energy Combust. Sci.* **2012**, *38*, 468–501.
- (46) Abtahizadeh, E.; de Goey, L. P. H.; van Oijen, J. A. Development of a novel flamelet-based model to include preferential diffusion effects in autoignition of CH₄/H₂ flames. *Combust. Flame* **2015**, *162*, 4358–4369.
- (47) Grandmaison, E. W.; Yimer, I.; Becker, H. A.; Sobiesiak, A. The strong-jet/weak-jet problem and aerodynamic modeling of the CGRI burner. *Combust. Flame* **1998**, *114*, 381–396.
- (48) Minamoto, Y.; Swaminathan, N.; Cant, R. S.; Leung, T. Reaction Zones and Their Structure in MILD Combustion. *Combust. Sci. Technol.* **2014**, *186*, 1075–1096.
- (49) Castela, M.; Veríssimo, A. S.; Rocha, A. M. A.; Costa, M. Experimental study of the combustion regimes occurring in a laboratory combustor. *Combust. Sci. Technol.* **2012**, *184*, 243–258.
- (50) Minamoto, Y.; Swaminathan, N. Scalar gradient behaviour in MILD combustion. *Combust. Flame* **2014**, *161*, 1063–1075.