NUMERICAL INVESTIGATION OF THE INFLUENCE OF OPERATING CONDITIONS ON A MILD LABORATORY SCALE COMBUSTOR

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Abstract

In this study, the numerical simulation of a small scale cylindrical combustor operating in the mild combustion regime is carried out. The fuel (methane) is supplied to the chamber through 16 nozzles placed around a central air nozzle. The operating power is equal to 10 kW. The simulations were performed using the commercial code Ansys Fluent with the k-ε realizable model for turbulence closure and the eddy dissipation concept for combustion modelling. The reaction mechanism comprises 19 species and 84 chemical reactions. A post-processing model for the prediction of NO has been used, taking into account the thermal, prompt and N_2O routes for NO formation. The effect of the excess air ratio and inlet air velocity on the temperature and mole fractions of CO, CO_2, O_2 and NO was studied. The influence of the air preheating temperature on the NO molar fraction was also investigated. The predictions are compared with comprehensive experimental data reported in the literature. It is shown that, in general, the model is able to provide good predictions, except in the vicinity of the burner where some discrepancies have been found, which is consistent with past work. The contribution of the prompt mechanism for the formation of NO is negligible, while that of the N_2O route is dominant for all cases investigated, even though the thermal mechanism becomes more important when the air preheating temperature increases.

Keywords: mild combustion, laboratory combustor, eddy dissipation concept, pollutant emissions

1. INTRODUCTION

Mild combustion has received significant and increasing attention in this century, due to the ability to significantly reduce NOx emissions in comparison to conventional combustion regimes. While in the latter there is a well-defined flame front, where the temperature becomes high enough to produce considerable amount of NO via the thermal mechanism, in the former the reaction zone is distributed and the average temperature is lower, as well as the temperature fluctuations. This mitigates the role of thermal NO, which is often dominant in practical combustion systems. Mild combustion is achieved by diluting combustion gases with the air or the fuel prior to combustion, by means of internal or external recirculation. The flame may be invisible, justifying the names of flameless or colourless combustion that are also commonly used to refer to this combustion regime. The air is often preheated to high temperature, leading to another common terminology, namely the high temperature air combustion.

Pioneering work on mild combustion was developed in the last decade of the 20th century [1-3], and in the beginning of this century [4-8], and the underlying theory and technology is described in Tsuji et al. [9]. Since then, significant progress has been made, and a few review articles are available [10-12].

Despite this, only a few works have reported comprehensive experimental data inside combustors, which are suitable for the assessment of predictive models. These include the work of Weber and co-workers [5, 7-8] in a 0.58 MW semi-industrial furnace of the Int. Flame Research Foundation; the experiments and simulations of Duwig et al. [13] in a model gas turbine combustor; the experiments of Costa and co-workers in a reverse flow small-scale combustor [14] and in two similar forward flow small lab-scale combustors equipped with different burners [15-19]; and the recent work of Lupant and Lybaert [20] in a lab-scale furnace whose temperature is controlled by sliding water-cooled tubes. Additional detailed experimental data are available for an unconfined jet in a hot diluted coflow, which emulates mild combustion conditions, e.g. [21-22].

In parallel with the previous studies, many computational works have addressed mild combustion, e.g., [5-8, 20, 23-26]. As far as the turbulence model is concerned, even though a few large eddy simulation (LES) studies have been reported, e.g. [27], most simulations have relied on the solution of the Favre-averaged Navier-Stokes equations using the standard, the RNG or the realizable k-ε models. In a few works, the Reynolds-stress model was also employed [24, 26].

In contrast to conventional combustion systems, which may be satisfactorily simulated assuming that chemistry is much faster than mixing, in mild combustion the chemical reactions are slower, due to the lower oxygen concentration in the reaction zone, so that the Damköhler number is of the order of unity [4, 23]. Therefore, flamelet models do not perform well, unless modifications are introduced, e.g., a formulation based on flamelet/progress variable [27-29]. The eddy dissipation concept (EDC), which may be used along with a detailed chemical mechanism, accounts for finite rate effects, has probably been the most widely used combustion model mild combustion simulations, with fair to good results [19-26], even though there is some evidence that the standard constants of the model may need modification [25, 29-31].

In the present work, the ability of the EDC model to predict the influence of changes in operating conditions (excess air, air preheating temperature, inlet air velocity) on the temperature and species concentrations fields is investigated using the detailed experimental data reported in Veríssimo et al. [16-17, 19]. Although the influence of the air preheating temperature was formerly reported [19], the NO predictions were not included, and so that they are presented here. The calculations were carried out using the commercial software Ansys-Fluent. Hence, the present results provide a useful insight on the predictive ability of models available in current commercial codes for mild combustion in a small scale laboratory combustor.

2. MATHEMATICAL MODELLING

The simulation model is based on the numerical solution of the Favre-averaged governing equations for mass, momentum and energy and on transport equations for the turbulence and combustion models. Turbulence was modelled using the realizable k-ε model [32]. This requires the solution of transport equations for the turbulent kinetic energy and its dissipation rate. Combustion was simulated using the EDC model [33], which is an improved version of the eddy dissipation model [34], allowing for detailed finite-rate chemical kinetics in the simulation of turbulent reactive flows. The transport equations for the species are solved during the CFD calculations.

The DRM-19 chemical mechanism [35], comprising 19 chemical species and 84 chemical reactions, was used. This is a reduced version of the GRI-1.2 full mechanism, and was developed to obtain the smallest set of reactions needed to closely reproduce the main combustion characteristics predicted by the full mechanism. It was formerly found, for a similar combustor, that the predictions obtained using the DRM-19 and the GRI-1.2 mechanisms were very close to each other [24]. Hence, the DRM-19 constitutes a good compromise between computational requirements and expected accuracy of the chemical mechanism.

Thermal radiation was calculated using the discrete ordinates method. The radiative properties of the participating medium were modelled using the weighted-sum-of-grey gases model.

When the chemical mechanism includes the nitrogen chemistry, the prediction of NO concentration may be carried out using the EDC model, e.g. [26]. Otherwise, the calculation of NO molar fraction may be predicted in a post-processing stage by solving a transport equation for NO mass fraction and using simplified models for the different NO mechanisms, e.g. [23-24]. The thermal, prompt and N2O mechanisms were considered in the present work, The NNH mechanism was found to be important in fuels containing nitrogen [36], and a few authors pointed out that the NO reburning mechanism also plays a role [37-39], but these routes were not considered in the present work.

The thermal NO formation was predicted using the extended Zeldovich mechanism, along with a quasi-steady-state assumption for the concentration of the nitrogen atom. The instantaneous concentrations of the oxygen and hydroxyl atoms were evaluated from the EDC model. The prompt NO formation was computed according to De Soete [40]. The formation of NO from molecular nitrogen via N_2O was considered by using a quasi-steady approximation. The mean reaction rates of NO were evaluated by integrating the instantaneous rate weighted by the pdf of the temperature and species, so that turbulent fluctuations are taken into account. The variance of temperature is estimated using an approximate algebraic expression derived from its transport equation by setting the production term equal to the dissipation term. An assumed clipped Gaussian pdf shape was used.

It is worth to point out that there are several options in the NO models (e.g., calculation method of the O and OH concentrations, quasi-steady vs. solution of transport equation for N_2O, the pdf shape, calculation method for the variance of the temperature) that have a non-negligible effect on the NO prediction. The options used were selected to improve the agreement with the experimental data for the calculations presented below.

3. LABORATORY COMBUSTOR

The combustion chamber is constituted by a quartz-glass cylinder with an inner diameter of 100 mm and a length of 340 mm, as shown in Fig. 1. The combustor is insulated with a 30-mm-thick ceramic fibre blanket. The burner is placed at the top end of the combustion chamber and the flue gases exit through a convergent nozzle at the bottom end. The burner consists of an air nozzle with an inner diameter of Dair nozzle=10 mm, through which the combustion air is supplied, surrounded by 16 small orifices of 2 mm inner diameter each, located on a circle with a radius of 15 mm, for the fuel (methane) supply. The combustion air is preheated up to Tair inlet = 700 ºC. The operating conditions are summarized in Table 1. The fuel thermal input and the inlet fuel velocity are maintained constant and equal to 10 kW and 6.1 m/s, respectively. Details on the experimental procedure may be found elsewhere [16-19].

Table 1:Operating conditions.

Case	$D_{air\ nozzle}$(mm)	λ	$T_{air\ inlet}$ (ºC)	V_{air} (m/s)
1	10	1.3	400	109.1
2	10	1.7	400	142.5
3	10	1.3	700	157.5
4	7	1.3	400	223.6

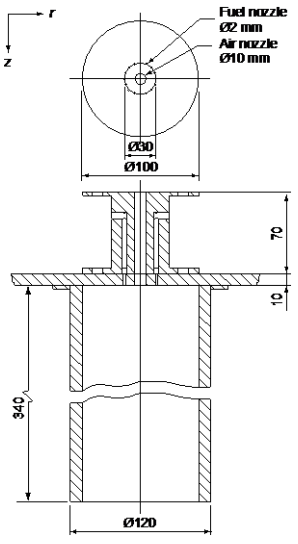

Figure 1. Schematic of the combustor

4. COMPUTATIONAL DETAILS

The computational domain is a section of 1/16 (22.5º) of the combustion chamber, with symmetry boundary conditions applied at the axial-radial boundary planes. Two different meshes were used with approximately 100,000 and 400,000 control volumes. The inlet fuel and air ducts were included in the computational domain, in order to allow the flow to develop and to reduce the uncertainty in the definition of the boundary conditions for the turbulent kinetic energy and dissipation rate at the entrance to the combustor. The grid is structured, except in the region of the fuel and air nozzles, with hexahedral control volumes over a large part of the computational domain, and non-uniform, being more refined close to the inlets and in the vicinity of the burner.

The comparison of the results for the two meshes showed that the difference between the predictions for the temperature and the species was marginal. In the case of NO molar fraction, differences between meshes in the range of 2-3 ppm were found. According to this analysis, the results presented below were obtained for the coarsest mesh.

Uniform axial velocity profiles of air and fuel were prescribed at the inlet section of the air and fuel ducts. The turbulent kinetic energy and the dissipation rate at the inlet were estimated following standard practices. Standard wall functions were used for the velocity boundary conditions at the walls of the combustor. The wall temperature was set to 1200 K. The emissivity of the solid boundaries was prescribed as 0.7. Pressure outlet with zero gauge pressure was set for the boundary condition at the exhaust.

The calculations were performed using the Ansys-Fluent commercial software. All the governing equations were solved using a second order upwind discretization scheme, and the SIMPLEC algorithm. The convergence criterion required that the sum of the residuals of the discretized equations over the domain decreased below 10^{-3}, except for the energy conservation equation, where a tolerance of 10^{-6} was used. In addition, it was checked that the values of the temperature and mass fractions of major species at several monitoring points of the computational domain, became approximately constant during the course of the iterative solution process.

5. RESULTS AND DISCUSSION

Figure 2 shows the predicted and measured radial profiles of temperature, and molar fractions of CO_2, O_2 and CO on a dry basis for two different values of the excess air coefficient (λ). Overall, and apart from the region in the vicinity of the burner, the

predictions are in rather good agreement with the experimental data of Veríssimo et al. [16]. There is a delay in the increase of temperature near the centreline, downstream of the burner, and the maximum temperature is overestimated at x=45 mm. This is consistent with the radial profiles of major species, which reveal that a slightly lower amount of CO_2 and CO, and higher concentration of O_2, are estimated at the centreline, x=45 mm, in agreement with the predicted low temperature in comparison with the measurements. Similarly, the maximum predicted temperature is related to an overestimation of CO_2 and CO, and an underestimation of O_2. The poor predictions of CO may be due to the limitations of the turbulence model, combustion model and/or chemical mechanism.

The influence of the excess air coefficient on the temperature and species concentration is rather well reproduced by the model, namely the lower temperature and concentration of CO_2, and the higher concentration of O_2 in the flue and recirculated gases experimentally observed with the increase of the excess air.

Measurements of the hydroxyl radical chemiluminescence revealed that the main reaction zone moves towards the burner as the excess air increases, leading to a conventional lean combustion regime and a visible flame for λ=1.7, in contrast to mild combustion for λ=1.3 [16]. This conclusion is hardly drawn from the measured and predicted temperature and species concentration profiles, even though the minor peak in the experimental radial temperature profiles at x=45 and 79 mm is typical of a conventional diffusion flame. The predictions reveal a temperature peak for both values of the excess air coefficient, but higher for λ=1.7. Moreover, the computed radial CO_2 profiles closer to the burner also exhibit a maximum for λ=1.7, while the corresponding O_2 profiles display a minimum.

The influence of the air preheating temperature (cases 1 and 3) is reported in Veríssimo *et al*. [19]. Therefore, we will now examine the influence of the inlet air velocity by changing the diameter of the air nozzle, while keeping the excess air coefficient unchanged. Figure 3 shows this effect by comparing the temperature and the species concentrations for cases 1 and 4.

The predictions of temperature and concentrations in the flue and recirculated gases are quite satisfactory, and exhibit a marginal dependence on the air velocity. However, discrepancies are found again downstream of the burner. The predictions of CO molar fraction are not good, even though the strong peaks observed in case 1 are strongly reduced in case 4. Overall, the calculations are closer to the experimental data in case 4 than in case 1.

The radial profiles of predicted and measured NO are presented in Fig. 4 for the various cases listed in Table 1. The predictions for case 1 are fairly good, with discrepancies found in the reaction zone, where there is almost no NO in the vicinity of the axis according to the predictions. In contrast, the measurements show that the NO molar fraction in that region is of the order of a few ppm, and increases radially more smoothly than in the predictions. An underprediction of about 5 ppm is observed at the last station (x= 310 mm).

The predictions for case 2 are a little better than for case 1. The NO molar fraction is larger when the excess air coefficient increases, except in the last two stations (x=250 and 310 mm), where an opposite trend was measured. This inversion was not computationally predicted, but the differences between the concentrations for cases 1 and 2 are rather small, both in the measurements and in the calculations.

The increase of the air preheating temperature causes a marked increase in the NO molar fractions, particularly away from the burner. This trend is correctly estimated by the model. Nevertheless, the predictions for case 3 are not satisfactory up to x=147 mm. While the measurements reveal that the radial evolution of the NO molar fraction is similar for cases 1 and 3, with higher values measured for case 3 in the recirculated flue gases, the predictions show negligible NO molar fraction downstream of the burner, and a strong radial increase at r = 0.10–0.15 mm.

The increase of the inlet air velocity from case 1 to case 4 yields a significant decrease of NO molar fraction and NO emissions. This effect is correctly estimated by the model, but the changes are relatively small in the predictions in comparison with the experiments.

The contribution of the various mechanisms of NO formation to the total predicted NO molar fraction was investigated by performing the calculations using only one mechanism while switching off the others. The results obtained are summarized in Fig. 5, which shows the axial NO profiles for the various mechanisms. The prompt mechanism has a negligible contribution in all cases, in agreement with the analysis reported elsewhere [16, 19, 36]. In all cases, the N_2O route for the formation of NO is dominant, particularly in cases 2 and 4, in which it contributes to more than 80% of the NO molar fraction.

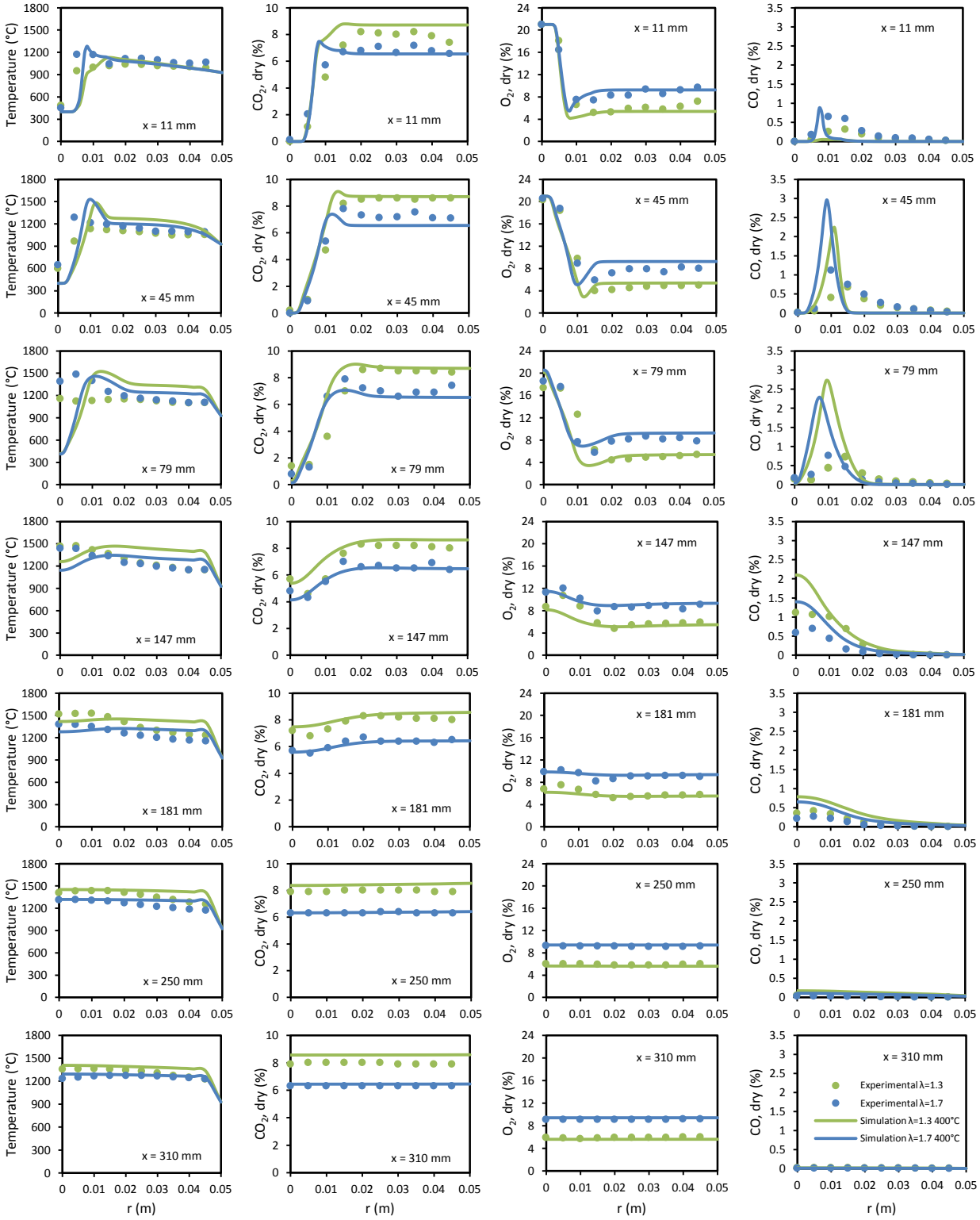

Figure 2. Radial profiles of temperature and species molar fractions for cases 1 and 2.

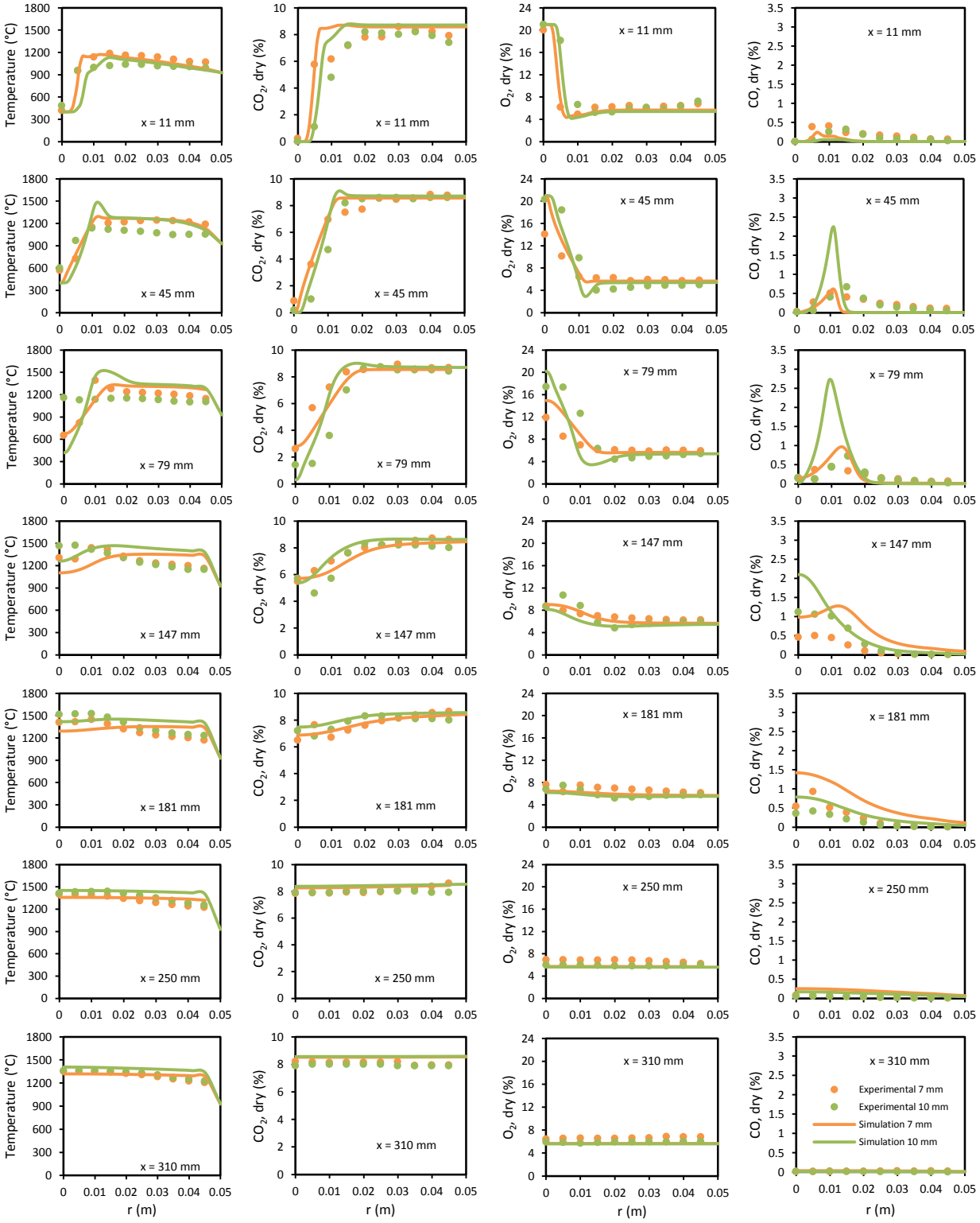

Figure 3. Radial profiles of temperature and species molar fractions for cases 1 and 4.

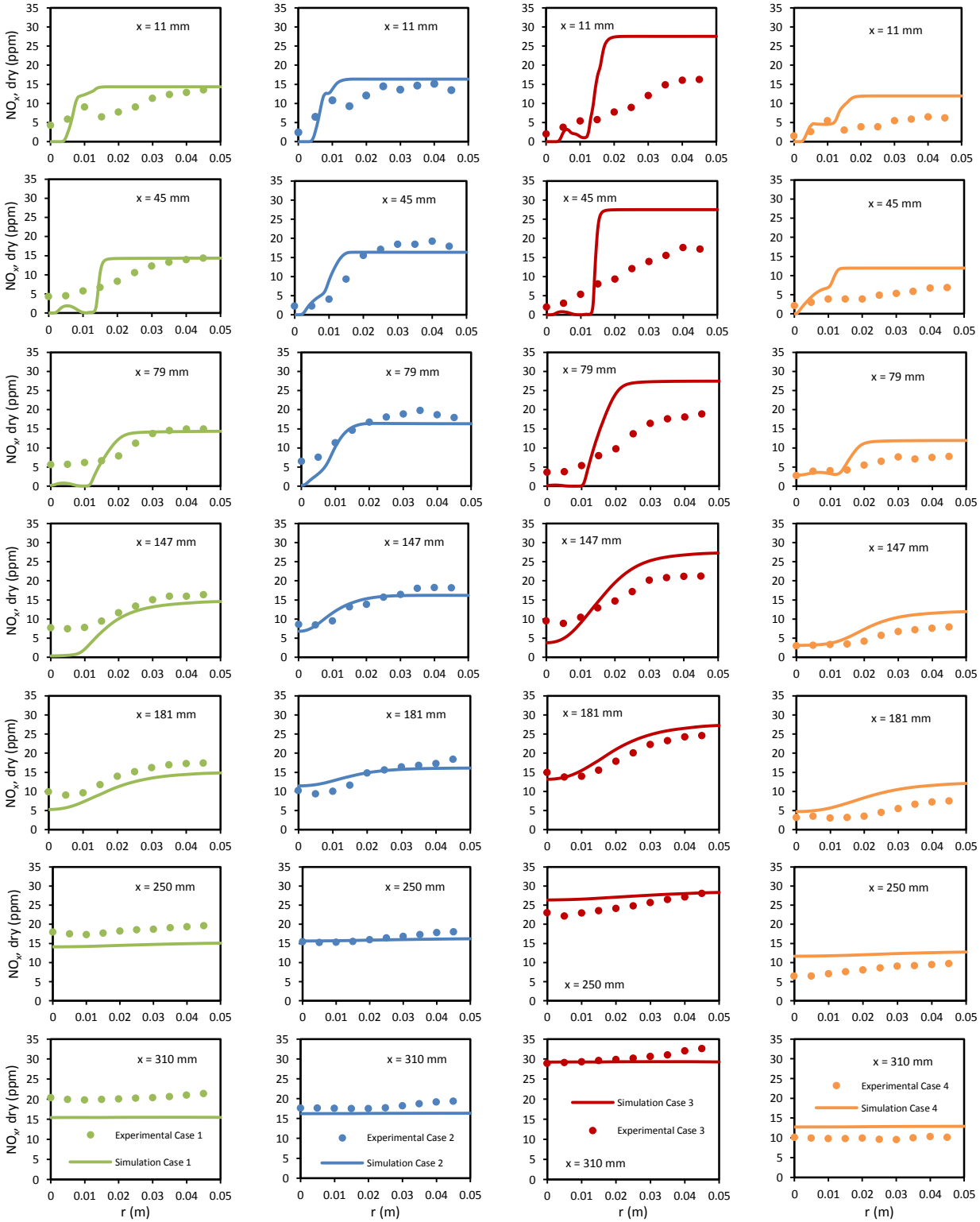

Figure 4. Radial profiles of NO molar fraction.

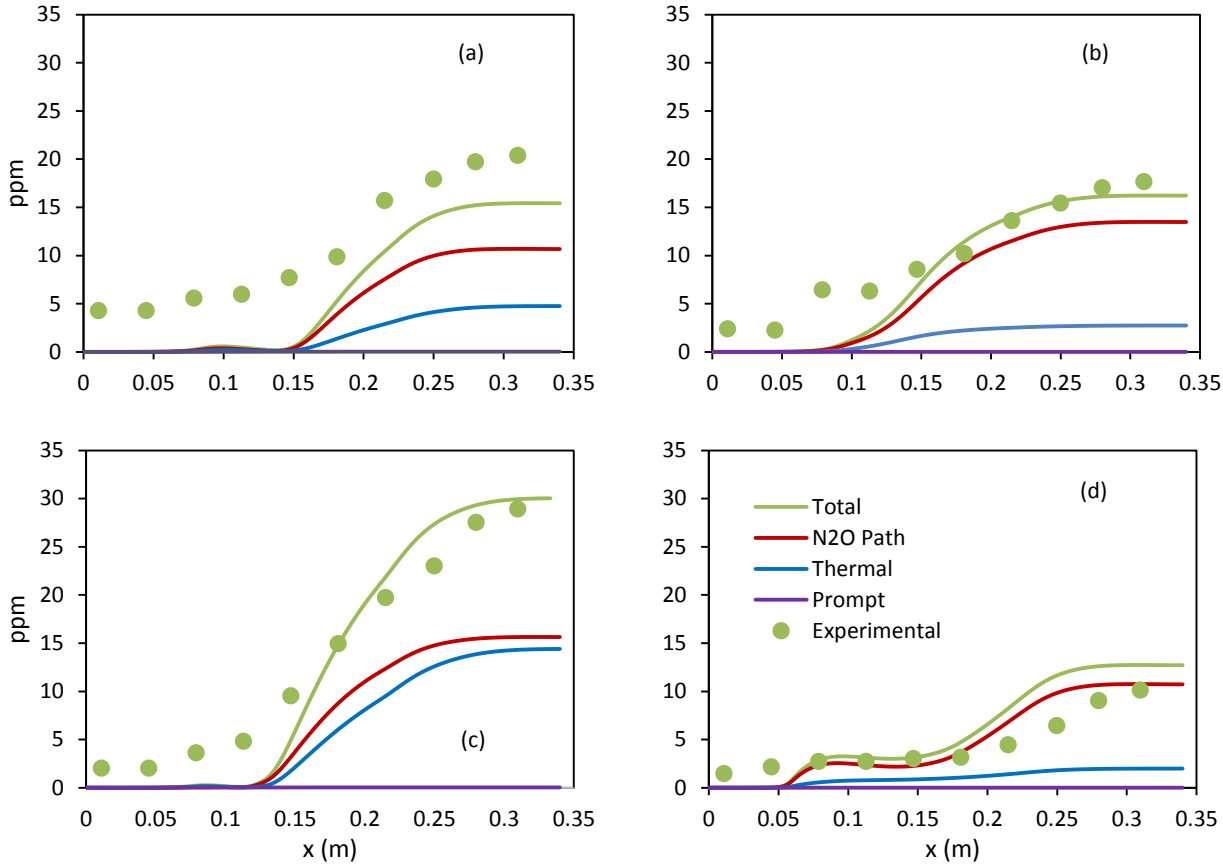

Figure 5. Contribution of the thermal NO formation mechanisms for the NO molar fraction along the centerline. (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4

Although there is a region close to the burner where the predicted temperatures are higher in case 1 than case 2, either the temperature is too low (x=11 mm) or the oxygen concentration is too small (x=45 mm) to form NO via the thermal mechanism. In case 3, the higher air preheating temperature is responsible for the existence of higher temperatures in the combustor, yielding a stronger contribution of the thermal mechanism, which becomes almost as important as the N_2O mechanism. In case 4, the temperatures are slightly lower than in case 1, reducing the role of the thermal mechanism.

6. CONCLUSION

A laboratory combustor operating in the mild combustion regime has been computationally simulated using the k-ε turbulence model and the eddy dissipation concept. The influence of the operating conditions on the combustion process has been investigated. The analysis carried out shows that the model is able to satisfactorily predict the temperature field and the molar fractions of CO_2 and O_2 in the combustor, except in the vicinity of the burner, where important discrepancies were observed. In general, the sensitivity of the model to changes in the operating conditions is satisfactory. The NO predictions are strongly dependent on the way the O and OH concentrations are evaluated, on the way the N_2O concentration is calculated, and on how the pdf is prescribed to determine mean values. The influence of the prompt mechanism is negligible, and the role of the N_2O for the formation of NO is dominant for all studied operating conditions. However, its relative importance becomes smaller with the increase of the air preheating temperature.

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