

Numerical Investigation of Flameless Combustion

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ABSTRACT

This article presents a numerical investigation of flameless combustion focusing on assessment of turbulence, combustion, and radiation modelling. The commercial code ANSYS FLUENT 19.0 is used to solve 3-D computational equations. Local measurements across a small lab cylindrical flameless combustor burning methane fuel were used for validation. Five different turbulence models were employed, namely realizable k- ϵ , shear stress transport k- ω (SST k- ω), RNG k- ϵ , Reynolds Stress Model (RSM) and transition SST. Results of RNG k- ϵ turbulence model were achieved a good agreement with the experimental data. The research focuses on assessment of several models for chemical kinetics and combustion simulations. Four numerical models were used namely Eddy Dissipation Concept (EDC), Finite-Rate/Eddy-Dissipation (FR/ED), combination of EDC with reduced mechanisms based on GRI-Mech 3.0 (GRI-EDC) and modified GRI-Mech 3.0. EDC combustion model was showed a good predication of mean temperature and mean dry basis volume fraction of O₂ and CO₂ emissions, but it cannot solve CO emissions. Generally, GRI-EDC was the best model for simulating the flameless combustion which have the ability to obtain better prediction of all characteristics. Moreover, the issue of radiation modelling was implemented, and results were compared in three cases, no radiation, P1 model and Discrete Ordinates (DO) radiation model. It was concluded that the radiation modelling does not yield significant differences in numerical prediction of mean temperature and species.

Keywords: *Flameless combustion; Turbulence; Combustion models; Radiation.*

1. Introduction

About three decades ago, the flameless combustion was identified to improve the combustion efficiency which reduces the harmful pollutants [1-3], hence achieve sustainability and reduce greenhouse effect. Flameless combustion is characterized by invisible chemical reaction zone, low CO and NO emissions, quiet and uniform temperature [3-6]. This combustion technology has several names such as HiTAC (High Temperature Air Combustion) [7], CDC (Colorless Distributed Combustion) [8,9], FLOX (Flameless oxidation) [3,10], MILD (Moderate or Intense Low-oxygen Dilution) [11-13], HiTOD (High-Temperature and Oxygen Deficient) [14] and HiCOT (High-temperature Combustion Technology).

Some of previous studies depends on preheated combustion air up to about 700 K or greater which helps in auto-ignition of reactants [3,6,15-20]. Moreover, internal exhaust gas recirculation has a significant effect on flameless phenomenon. Therefore, combustion air commonly injected with high velocity approximately 90 m/s [21]. Verissimo et.

al. [22] used different air nozzle diameters to study the significance of air injection velocity to flameless combustor. It was found that increasing the inlet air velocity participates in reactants dilution with recirculated hot combustion products. Yang and Blasiak [14] investigated the influence of preheated air temperature and oxygen concentration on flameless combustion and jet entrainment rates. It was found that decreasing the oxygen concentration leads to an increase in jet entrainment subsequently, larger uniformity of heat release.

Rebola et. al. [16] performed an experimental investigation of flameless combustor characteristics. The results showed that flameless combustor has a wide range of operating conditions. Verissimo et. al. [17] presented an experimental and computational study for the effect of preheated air temperature on methane flameless combustor characteristics. Global EDC and Skeletal mechanisms were compared for combustion modelling. Radiation effect was taken in concern using Discrete Ordinates (DO) model. Turbulence was simulated using Realizable k- ϵ

equations. The results showed a good agreement between computational and experimental measurements. Kumar et. al. [23] reported an experimental and computational study of a new burner design which uses combustion air at ambient temperature. Flameless mechanism was depending on the geometrical design of burner which achieve high recirculation ratio. Some of results were showed that it is not a mandatory to preheat combustion temperature for flameless creation as reported by Paul et al [24] and Craig et al [25]. Also, it was found that Soot formation can be negligible in flameless combustion [24]. Coelho et. al. [26] simulated numerically flameless combustion using standard k- ϵ model and laminar flame let model. Preheated air temperature with high recirculation ratio was employed. The results showed a good agreement between predicted and measured velocity. Eddy dissipation concept [19] and RSM and realizable k- ϵ were used in flameless simulations [27]. Large eddy simulation was performed by Duwig et. al. [28] for computational calculations of flameless combustion in gas turbines. Galletti et. al. [29] carried out an experimental and numerical study of flameless burner. Combustion modeled using the combined eddy dissipation model/finite rate chemistry (EDM/FRC). CFX and standard k- ϵ model with varying the first constant of dissipation transport equation from 1.44 to 1.6 to improve the prediction of round jets. Thermal NO formation was simulated using a finite rate chemistry combustion (FRC) model and a simplified one-step kinetic mechanism. Effect of excess air and air inlet velocity were studied and degree of recirculation was obtained. Mancini et. al. [30] simulated the combustion using standard k- ϵ model and RNG k- ϵ model. It was concluded that the failing of RANS models in simulating the physics of the fuel jet was a result of error in predictions of the entrainment subsequently, it is not related to any chemistry sub-models.

In spite of the valuable researches on the CFD investigation of flameless combustion regime, some fundamentals related to turbulence, combustion and radiation still not investigated clearly with in one comparison study. The main purpose of this paper is to introduce a numerical investigation of flameless combustion focusing on assessment of turbulence, combustion and radiation modelling. Five different turbulence models were employed, namely realizable k- ϵ , shear stress transport k- ω (SST k- ω), RNG k- ϵ , Reynolds Stress Model (RSM) and transition SST. The research focuses on assessment of several models for chemical kinetics and combustion simulations. Four numerical models were used namely Eddy Dissipation Concept (EDC), Finite-Rate/Eddy-

Dissipation (FR/ED), combination of EDC with reduced mechanisms based on GRI-Mech 3.0 (GRI-EDC) and modified GRI-Mech 3.0. The issue of radiation modelling to be studied in three cases, no radiation, P1 model and Discrete Ordinates (DO) radiation model.

2. Geometrical Configurations

Figure (1) shows the burner and combustor configuration which were used in the present numerical study. Experimental details and results were reported in details by Verissimo et al. [17,31]. A 100 mm diameter insulated quartz-glass cylinder with 340 mm length was used. Combustor outlet section is a steel tapered cylinder with angle 15°, 150 mm length as shown in Figure (2). A 30 mm thickness ceramic fiber blanket was used for combustor insulation and to maintain the wall at high temperature. Co-axially flameless burner configuration has one air inlet nozzle (d=10 mm) located at the center of the burner, which is surrounded by 16 fuel nozzles (d=2 mm) arranged on a 30 mm diameter circle as shown in Figure (1). Methane (natural gas) fuel was utilized at ambient temperature. The combustion air was supplied and preheated up to 700°C. Due to the symmetrical configuration, a half section was used to reduce the CFD cost.

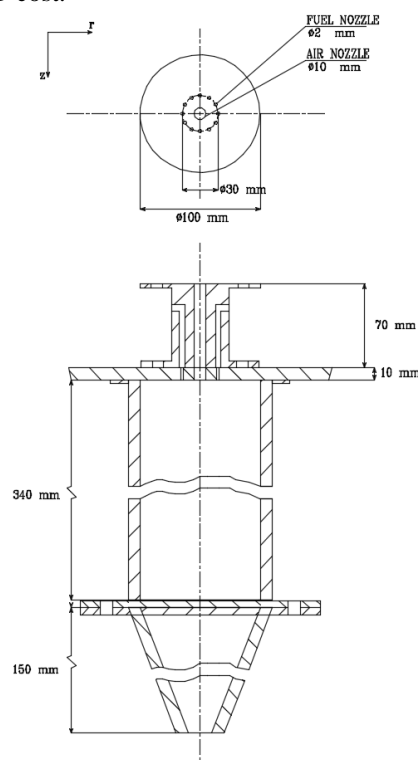


Figure 1 Schematic drawing of the combustor (Verissimo et al. [17,31])

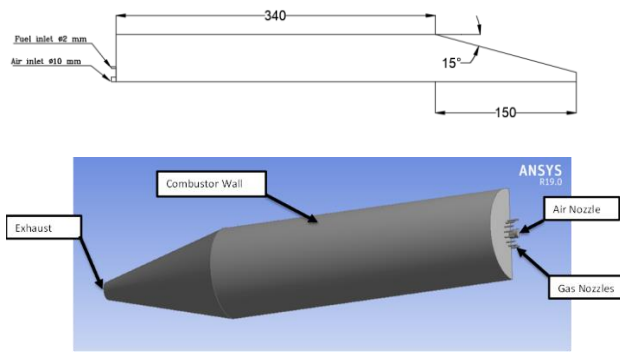


Figure 2 Detailed dimensions of the combustor with exhaust section and 3D configuration

3. Mathematical Modeling

A three-dimensional (3D) configuration of flameless combustor was modeled using ANSYS Fluent V19.0. A finite volume technique was used to compute the governing equations for mass, energy and momentum equations. Steady state, pressure-based solver was defined in the present work. Simple pressure velocity coupling was employed, second-order upwind schemes and SIMPLEC algorithm were used in discretization of governing equations. 3-D geometry was created using ANSYS design modeler. Fine structured mesh was generated and employed using ANSYS Meshing as shown in Figure (3). It seems obvious that the grid size was refined near to wall of combustor, inlet air and inlet fuel sections. Five different turbulence models were employed in the present research, namely realizable k- ε, shear stress transport k-ω (SST k-ω), RNG k- ε, Reynolds Stress Model (RSM) and transition SST for selecting the most applicable model. In the current simulation, the issue of radiation modelling was studied and results were compared in three cases, no radiation, P1 model and Discrete Ordinates (DO) radiation model. Combustion modelling based on integration of energy equation has been investigated in FLUENT theory guide [32]. Eddy-dissipation concept (EDC) model was used for modelling turbulence and chemistry interaction in the current simulation. EDC was not able to predict all species of combustion so, the detailed chemical reaction mechanism GRI-MECH 3.0 of 53 chemical species and 325 reactions or reduced mechanism of GRI can be used with EDC. In this paper, EDC with GRI-MECH 3.0 of 53 chemical species was employed to predict CO and NOx emissions.

4. Computational Model

All setting of present simulation can be summarized as shown in **Table (1)**. To evaluate the solution convergence, the scaled residuals were lower than 10^{-3} , except for energy residuals were lower than 10^{-6} .

Three mesh sizes (G1: 1 million, G2: 1.6 million G3: 2.8 million) were considered for the purpose of grid independency study. G1 was used in the current simulation with Y^+ value about 30 for standard wall function. Boundary conditions shown in **Figure (4)** and their specs listed in **Table (2)**.

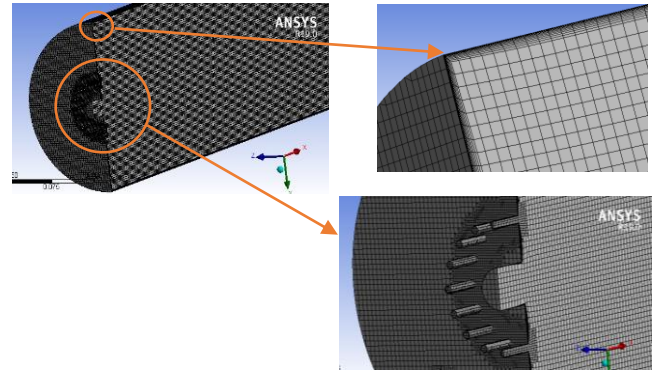


Figure 3 Computational domain meshing and grid of flameless combustor (half-section) with focusing on burner section and wall inflation.

Table 1- Simulation specifications

Viscous model	Case 1: K-ε realizable Case 2: SST k-ω Case 3: RNG K-ε Case 4: RSM Case 5: RNG
Near wall modelling	Standard wall function
Radiation model	Case 1: No Radiation Case 2: DO Case 3: P1
Combustion model	Species transport model
Mixture properties	Methane-air
Turbulence chemistry interaction	Case 1: EDC Case 2: EDC&GRI 3.0 Case 3: FR-ED Case 4: Modified GRI-EDC
Reaction	Volumetric

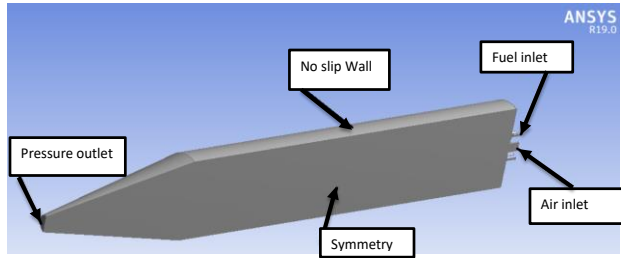


Figure 4 Operating boundary conditions

Table 2 Simulation boundary conditions

Oxidizer (Air) inlet	Velocity	157.5	m/s
	Gage pressure	0	Pa
	Temperature	973	K
	Hydraulic diameter	10	mm
	Oxygen mass fraction	0.23	
	Turbulence intensity	20	%
Fuel inlet (Methane)	Velocity	6.1	m/s
	Gage pressure	0	Pa
	Temperature	300	K
	Hydraulic diameter	2	mm
	CH4 mass fraction	1	
	Turbulence intensity	20	%
Stationary wall (combustor)	Wall slip	Non-slip	
	Thermal condition	Fixed	
	Temperature	1400	K
Pressure outlet	Hydraulic diameter	196	mm
	Gage pressure	0	Pa
	Turbulence intensity	10%	

5. Results and Discussion

A grid independency study was performed to evaluate the mesh and to select the proper computational grid with smallest error. Three grids were used 1 million, 1.6 million and 2.8 million as presented in Figures (5 and 6). The numerical predicted radial profiles of the mean temperature, CO₂ and O₂ were validated with the experimental at six axial locations ($X/L = 0.022, 0.091, 0.161, 0.432, 0.369$ and 0.510) respectively. Results of 1.6 million grid was showed a reasonable agreement with relatively low running time.

The significance of radiation modelling on the numerical solution of flameless combustion was studied. The predictions of three cases for radiation modelling: DO model, P1 Model and without taking radiation in consideration was investigated. Figures (7 and 8) presented the numerical predicted radial profiles of the mean temperature, CO₂, CO and O₂ were showed at eight axial locations ($X/L = 0.022, 0.091, 0.161, 0.23, 0.432, 0.369, 0.510$ and 0.632) respectively at the three cases of radiation modelling for the same turbulence (RNG k- ϵ) and combustion (GRI-EDC) models. The predictions of three cases showed similar trends with very low differences. Overall, taking radiation in modelling can be neglected as shown in the predicted results and because of most of exhaust gases contains non luminous gases such as CO₂ and H₂O. Also, the flameless combustion may be considered as a complete combustion which means no soot formation in the combustion products therefore no luminous combustion regime. Subsequently, radiation was very low in flameless combustion and can be neglected in the modelling. Figure (9) shows the numerical predicted axial profiles of the mean temperature, CO₂, CO and O₂ for the three cases of radiation modelling and showed the same conclusions. The predictions of different five turbulence models were employed, namely realizable k- ϵ , shear stress transport k- ω (SST k- ω), RNG k- ϵ , Reynolds Stress Model (RSM) and transition SST. Figures (10 and 11) demonstrated the numerical predicted and measured radial profiles of the mean temperature and mean dry basis mole fraction of CO₂, CO and O₂ at eight axial locations ($X/L = 0.022, 0.091, 0.161, 0.23, 0.432, 0.369, 0.510$ and 0.632) respectively for different turbulence models. Results showed that most of models fails to predict the temperature at near burner region (At $X/L = 0.022, 0.091, 0.161$) due to the high turbulence and intensive mixing. RSM model was recommended for the studies which interested in with near burner modelling, but it was overestimated prediction at the remote area where the remaining studied models were preferred. Also, RSM was achieved better agreement with the experimental results of CO₂ mole fraction prediction radial profiles along the combustor centerline. Both of two models, realizable k- ϵ and RNG k- ϵ shows relatively similar trends. Generally, these two models recommended for flameless combustion modelling, but RNG k- ϵ shows the best agreement with the experimental results.

Figure (12) shows the predicted flow streamlines through the combustor. It is noticed that the recirculated combustion products covered large volume of the combustor which comes from high air velocity at the center. This leads to a high mixing and

turbulence near the burner tip as shown in Figure (13), subsequently high dilution of the mixture and low O₂ content. This dilution leads to a decrease in reaction rate which permits to wide distributed reaction zone and hence, uniform temperature distribution along the combustor as shown in Figure (14). The previous studies shows that the flameless combustion occurs at high recirculation ratio. Recirculation ratio was defined as the ratio between recirculated combustion products flow rate and the inlet reactants flow rate. The predicted recirculation ratio for the current case was calculated at the center of vortex as shown in Figure (15) and was found to be 2.94. Figure (15) shows the axial velocity contour and the yellow region refer to the negative velocity which represent the recirculated gases.

The combustion was modelled using different mechanisms, Eddy Dissipation Concept (EDC), Finite-Rate/Eddy-Dissipation (FR/ED), combination of EDC with reduced mechanisms based on GRI-Mech 3.0 (GRI-EDC) and modified GRI-Mech 3.0. Radial prediction of mean temperature and dry volume fraction of O₂, CO₂ and CO were investigated in Figures (16 and 17). The over estimation of all models for predicted mean temperature and emissions may be due to in accurate description of wall emissivity or any other factors such as fixed wall temperature which may be vary through the experimental work. The wall temperature, or actually the wall heat loss may indeed be a relevant factor in that deviation and over estimation. Both of two models GRI-EDC and Global EDC leads to a relatively good estimation for all studied results. FR-EDC model results illustrated greater discrepancies and was the worst prediction for

mean temperature and dry volume O₂ concentration particularly, at near burner region (recirculation zone) at four axial locations ($X/L = 0.022, 0.091, 0.161$ and 0.23). It was noticed that FR/EDC yields peak in the radial temperature and CO₂ profiles at near burner region (at axial locations $X/L = 0.022, 0.091$ and 0.161). This peak temperature appeared as a result of too early ignition.

The deviations in the temperature in the near burner field may well be due to the fact that the models that have been used do not incorporate an accurate representation of the turbulent fluctuations in mixing. This is offered by other models incorporating equations for mean and variance of mixture fraction. Modifications of EDC model constants which called volume fraction constant C_{ξ} and time scale constant C_{τ} were done to reduce this peak. These constants were changed from 2.1377 and 0.4082 to 5 and 0.2 respectively and leads to slightly earlier in ignition and reducing the peak of mean temperature as shown in Figures (16 and 17) (at axial locations $X/L = 0.091$ and 0.161). This modification was called as Modified GRI-Mech which shows a good prediction for axial mean temperature and dry volume fraction of O₂, CO₂ and CO as shown in Figure (18). It was noticed that Modified GRI-Mech has the best estimation for Axial CO prediction, but it wasn't the best as an overall detailed radial prediction as displayed in Figures (16 and 17). Overall, it was observed from the radial and axial prediction that GRI-EDC model was the more accurate prediction.

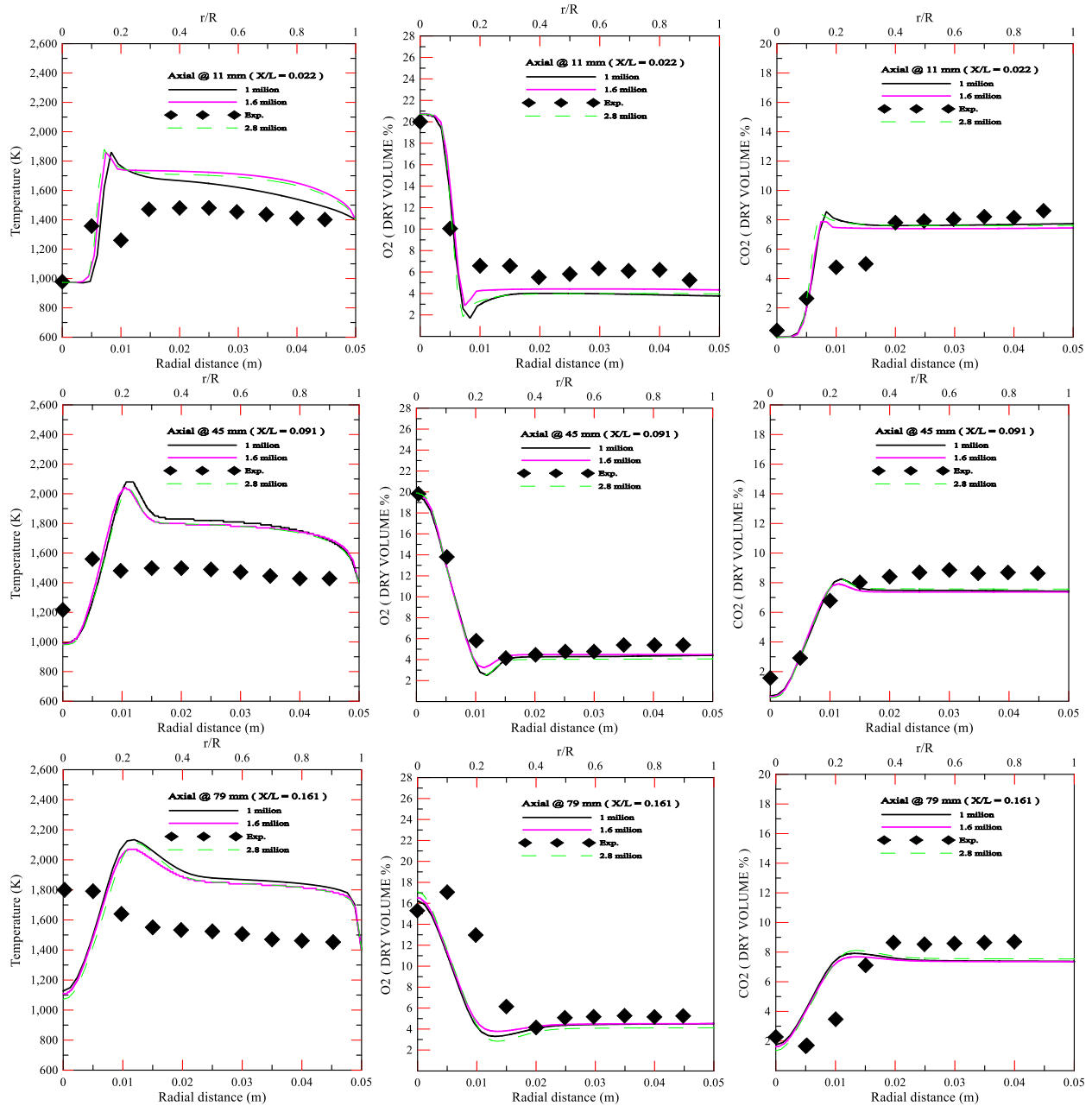


Figure 5 The numerical predicted radial profiles of the mean temperature, CO₂ and O₂ were validated with the experimental at three axial locations ($X/L = 0.022, 0.091$ and 0.161) respectively

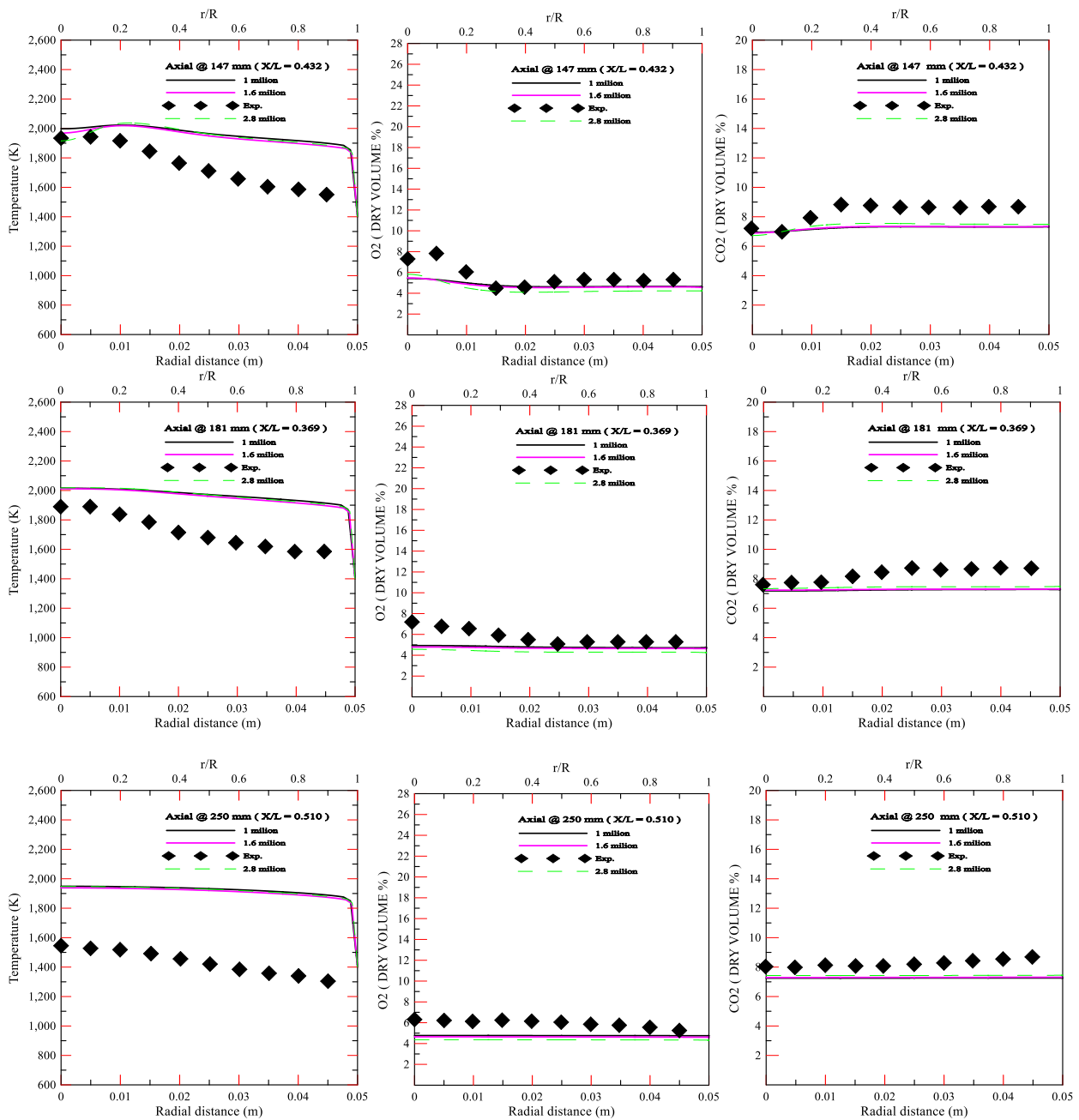


Figure 6 The numerical predicted radial profiles of the mean temperature, CO₂ and O₂ were validated with the experimental at three axial locations ($X/L = 0.432, 0.369$ and 0.510) respectively

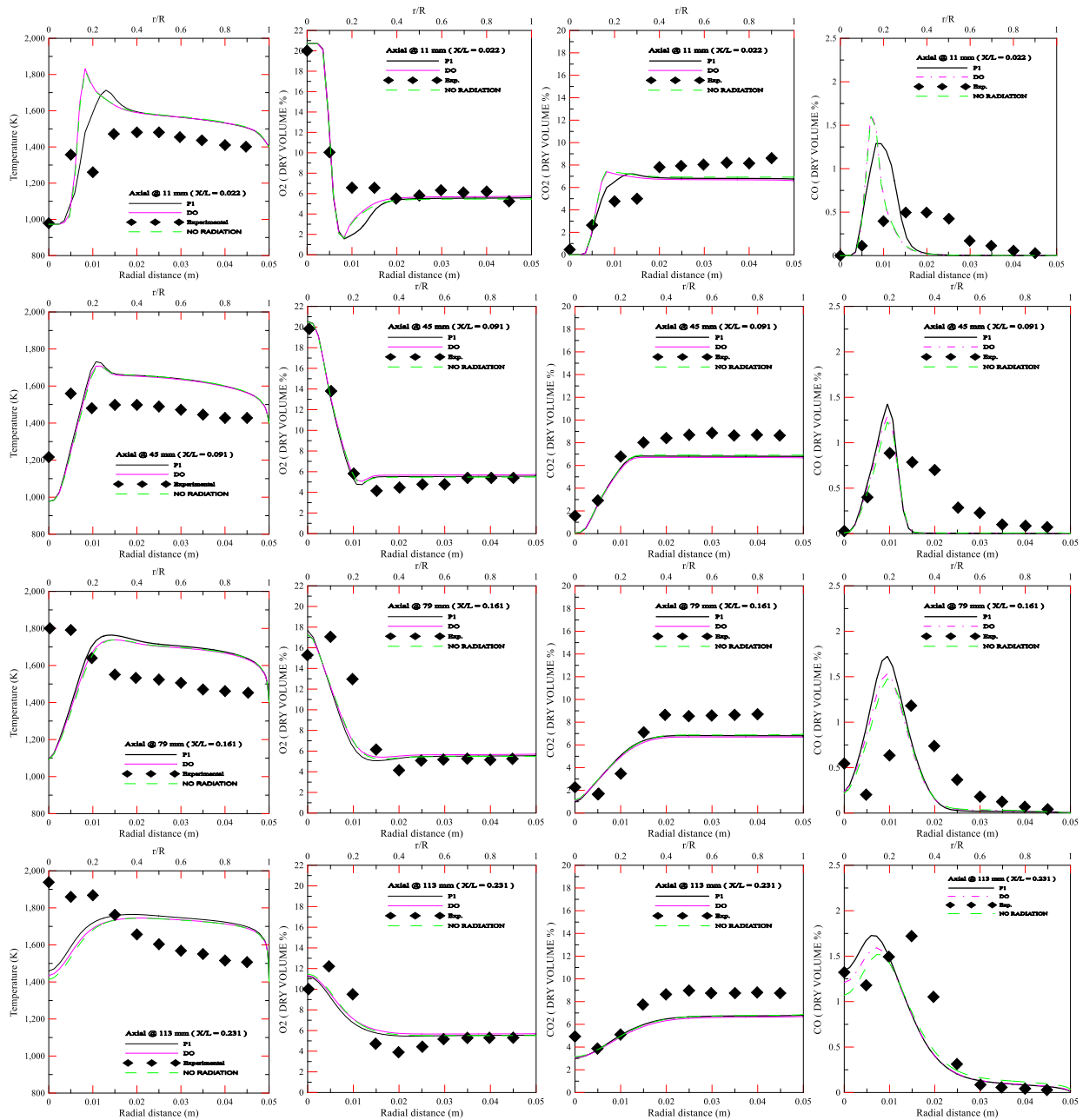


Figure 7 Predicted and measured radial profiles of mean temperature and dry volume fraction of CO₂ and O₂ at four axial locations (X/L = 0.022, 0.091, 0.161 and 0.231) respectively at different radiation modelling

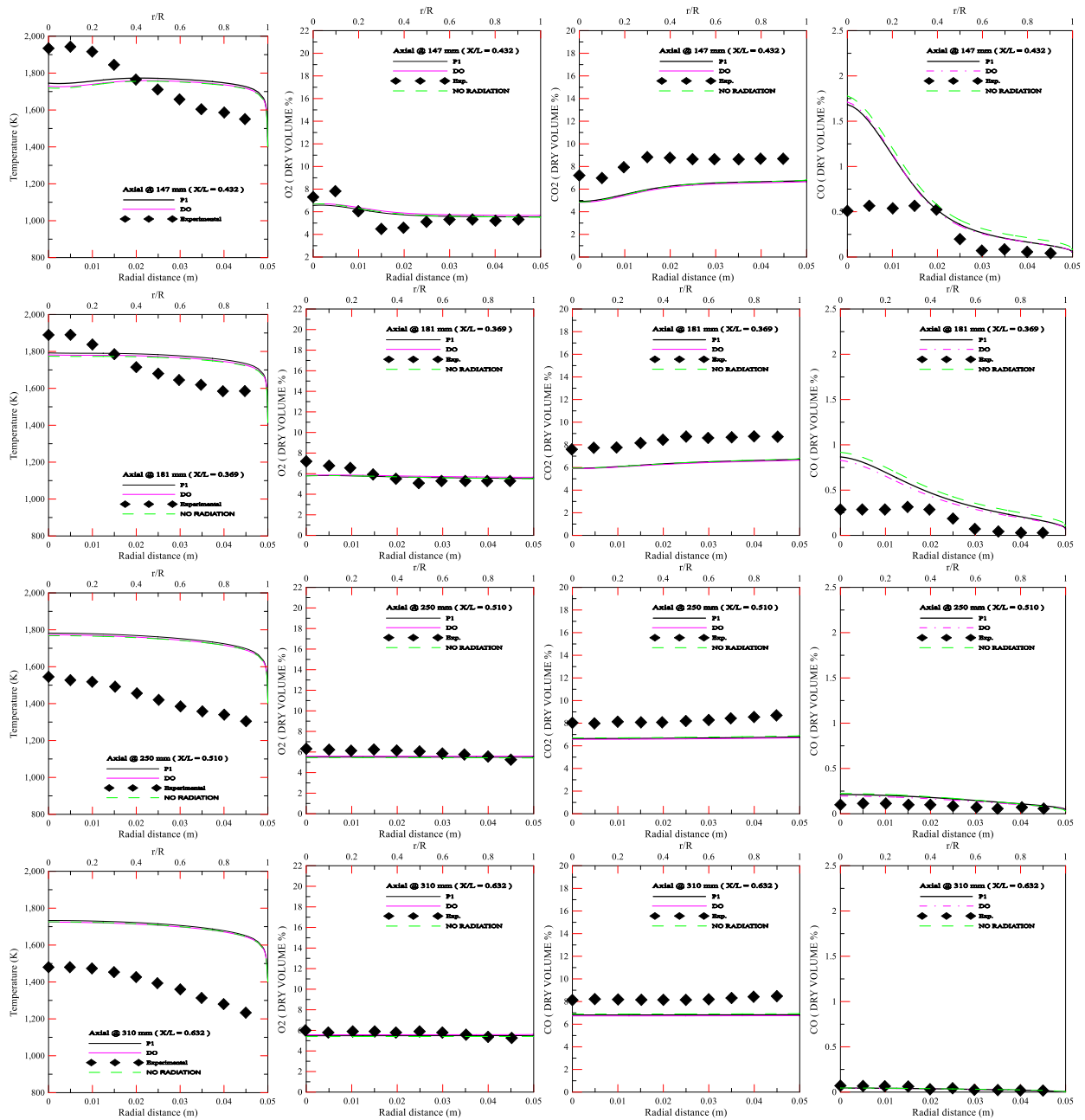


Figure 8 Predicted and measured radial profiles of mean temperature and dry volume fraction of CO₂ and O₂ at four axial locations (X/L = 0.432, 0.369, 0.510 and 0.632) respectively at different radiation modelling

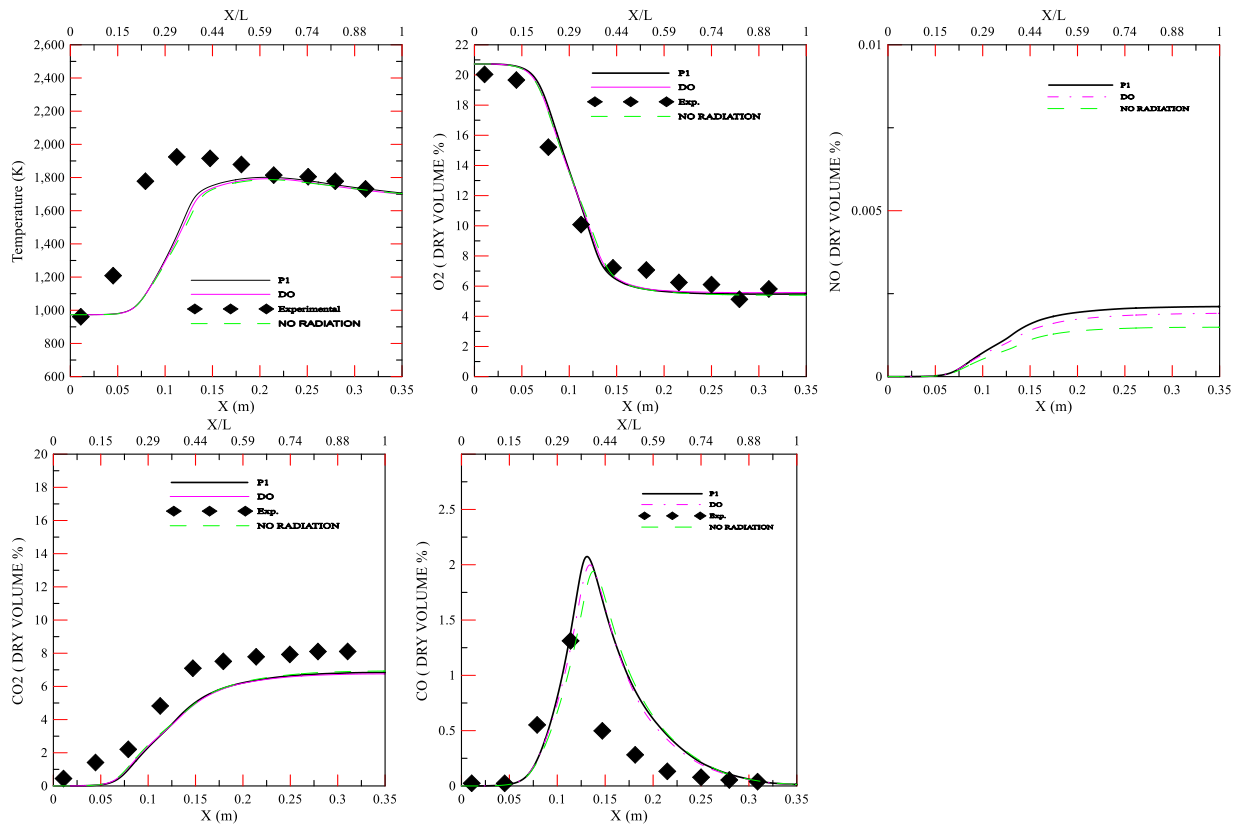


Figure 9 Predicted and measured axial profiles of mean temperature and dry volume fraction of CO₂ and O₂ at different radiation modelling

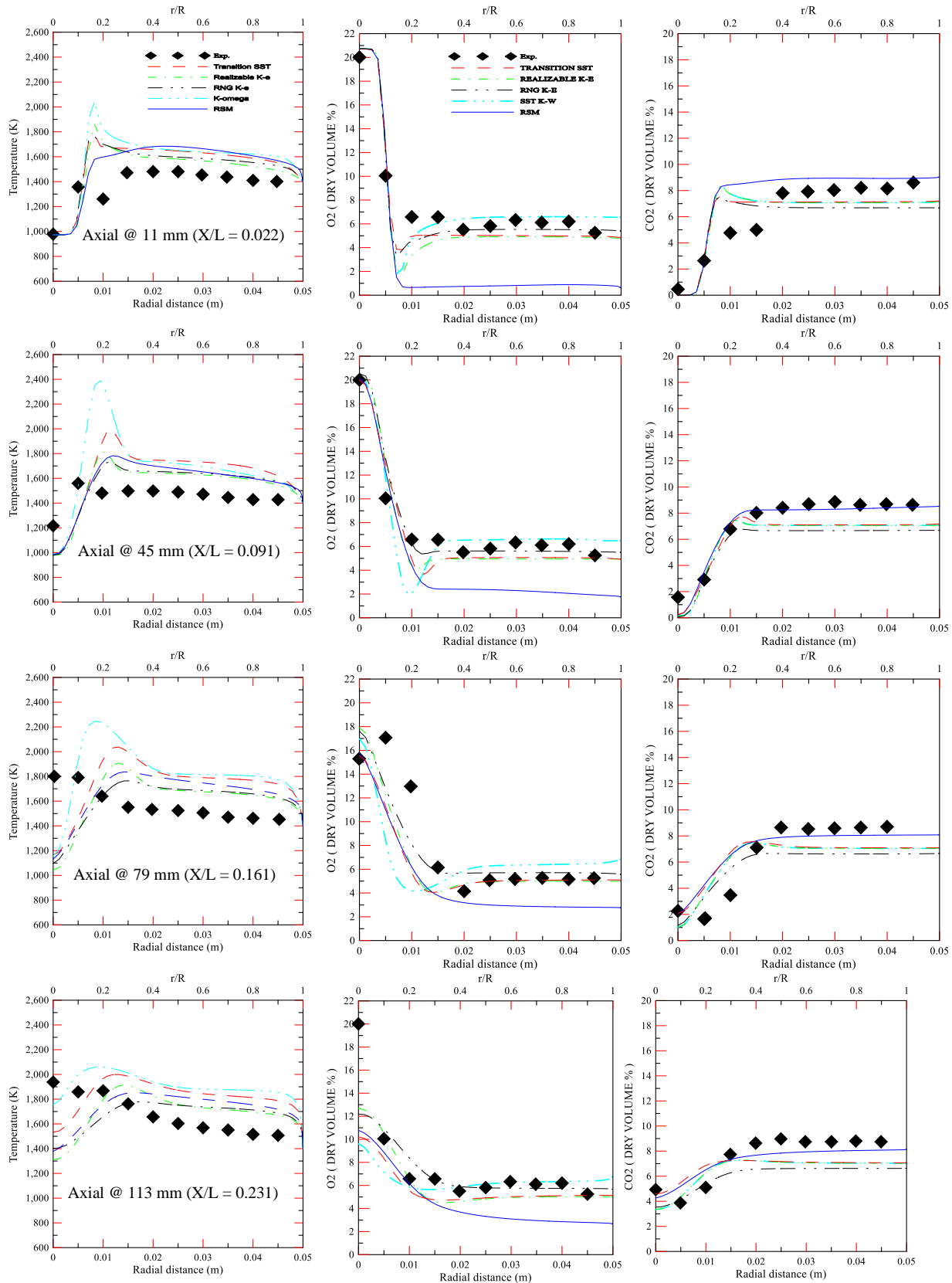


Figure 10 Predicted and measured radial profiles of mean temperature and dry volume fraction of CO₂ and O₂ at

four axial locations ($X/L = 0.022, 0.091, 0.161$ and 0.23) respectively at different turbulence modelling

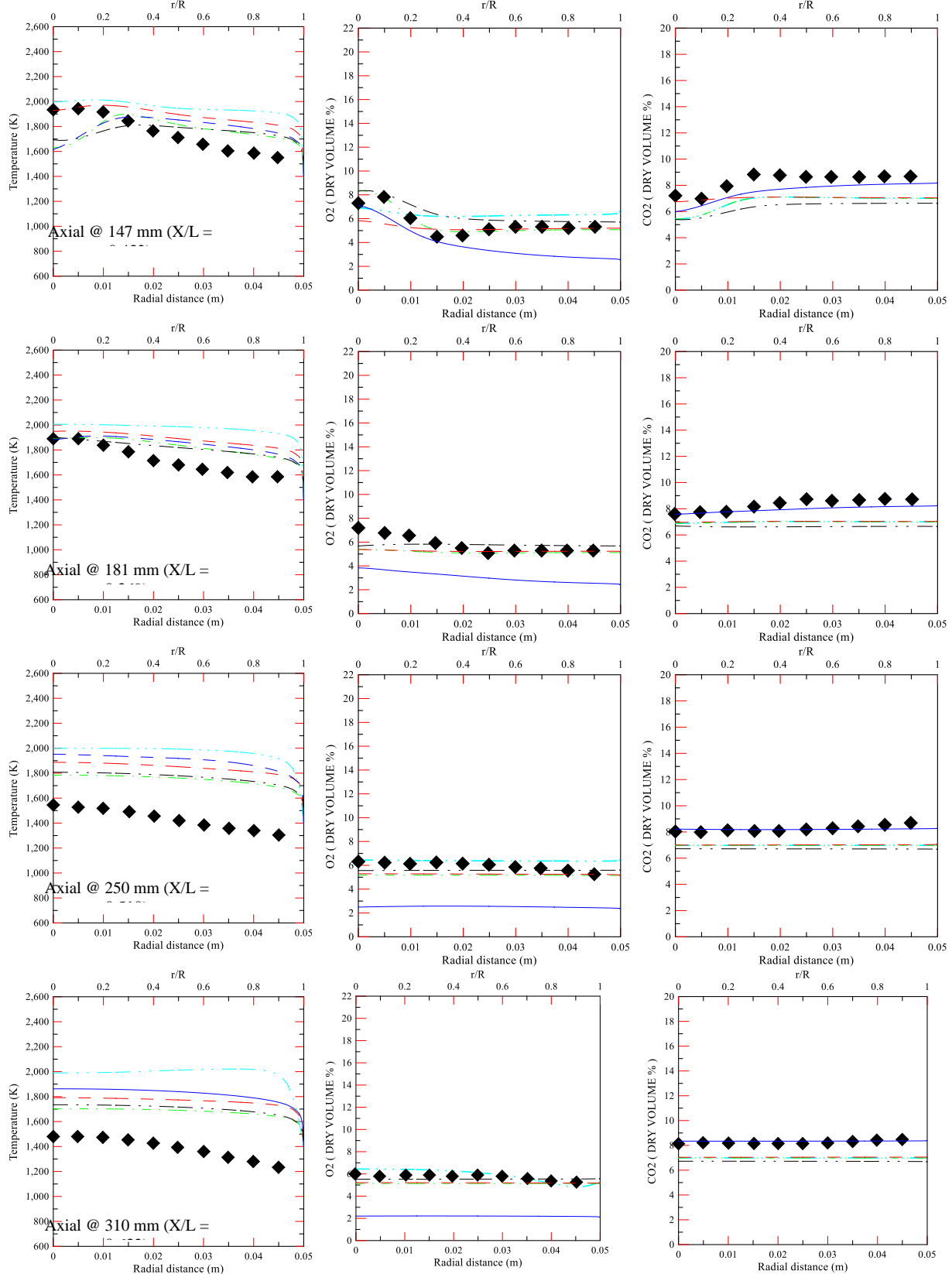


Figure 11 Predicted and measured radial profiles of mean temperature and dry volume fraction of CO_2 and O_2 at

four axial locations ($X/L = 0.432, 0.369, 0.510$ and 0.632) respectively at different turbulence modelling

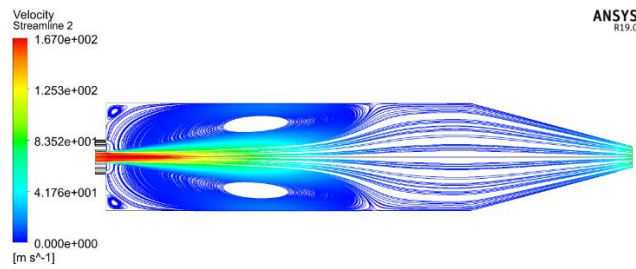


Fig. 12 Predicted flow streamlines through the combustor symmetry plane

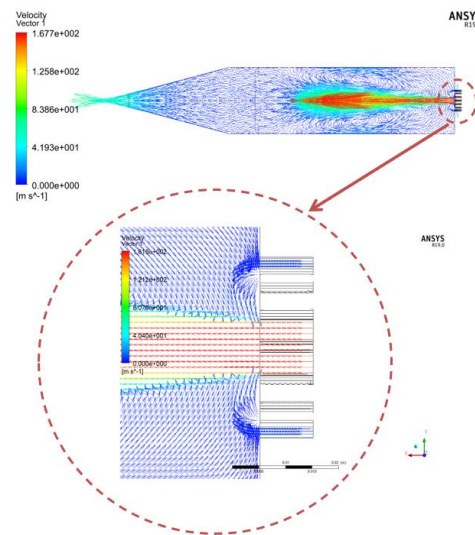


Figure 13 Predicted mean velocity vectors through the combustor symmetry plane

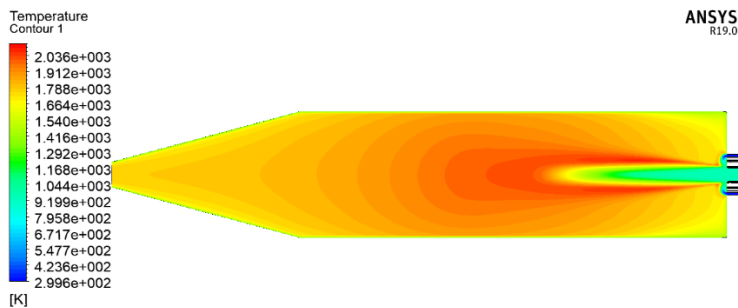


Figure 14 Predicted contours of mean temperature through the combustor symmetry plane

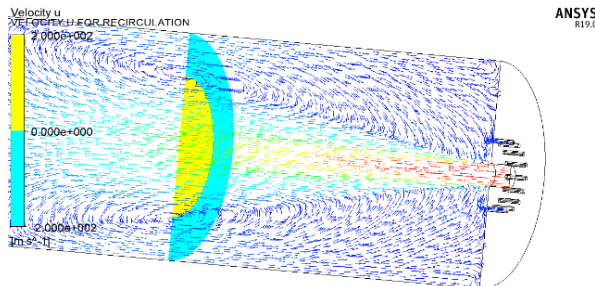


Figure 15 Velocity contours at plane of calculated recirculation ratio located at vortex center

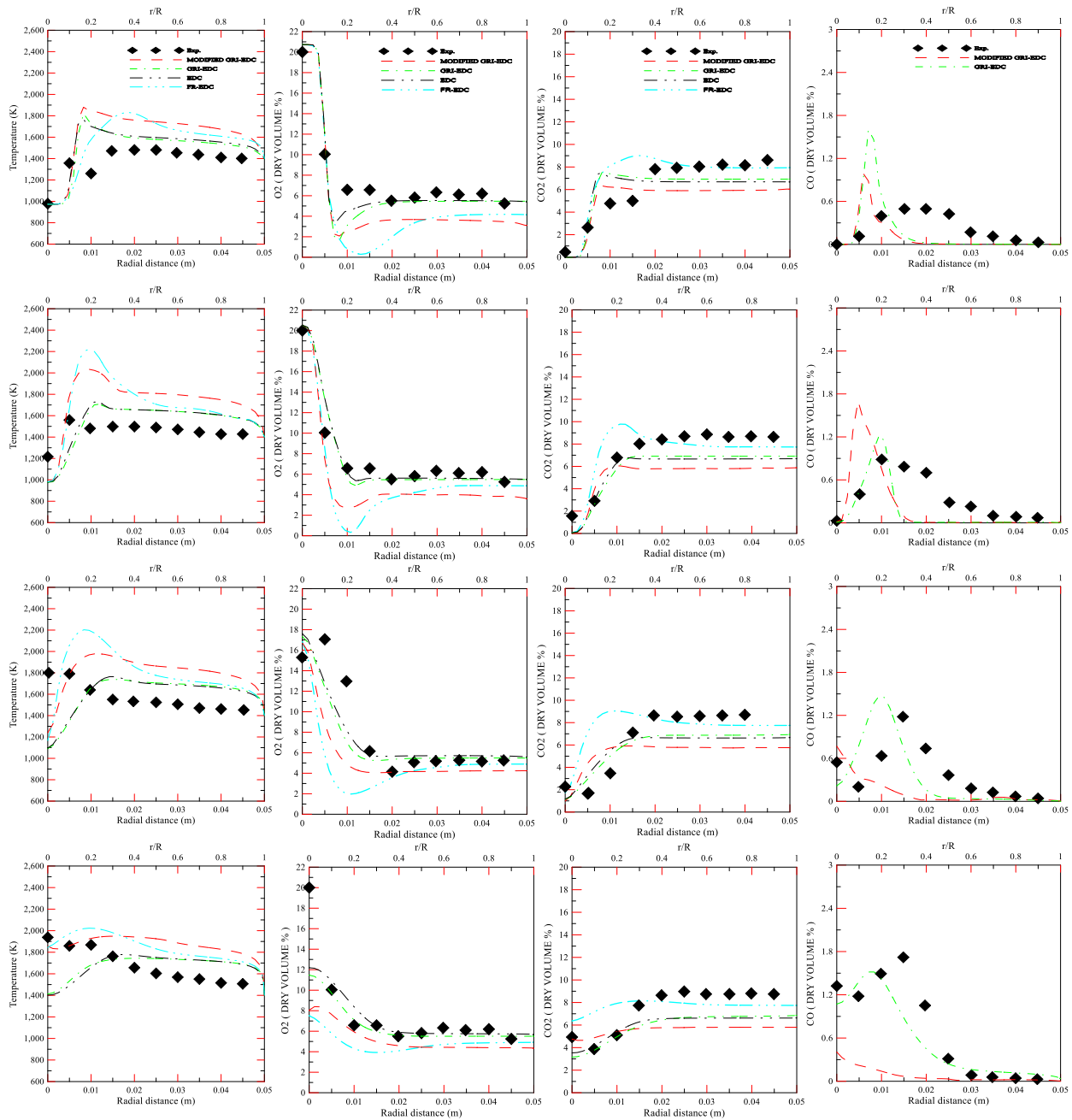


Figure 16 Predicted and measured radial profiles of mean temperature and dry volume fraction of CO₂ and O₂ at four axial locations (X/L = 0.022, 0.091, 0.161 and 0.23) respectively at different combustion modelling

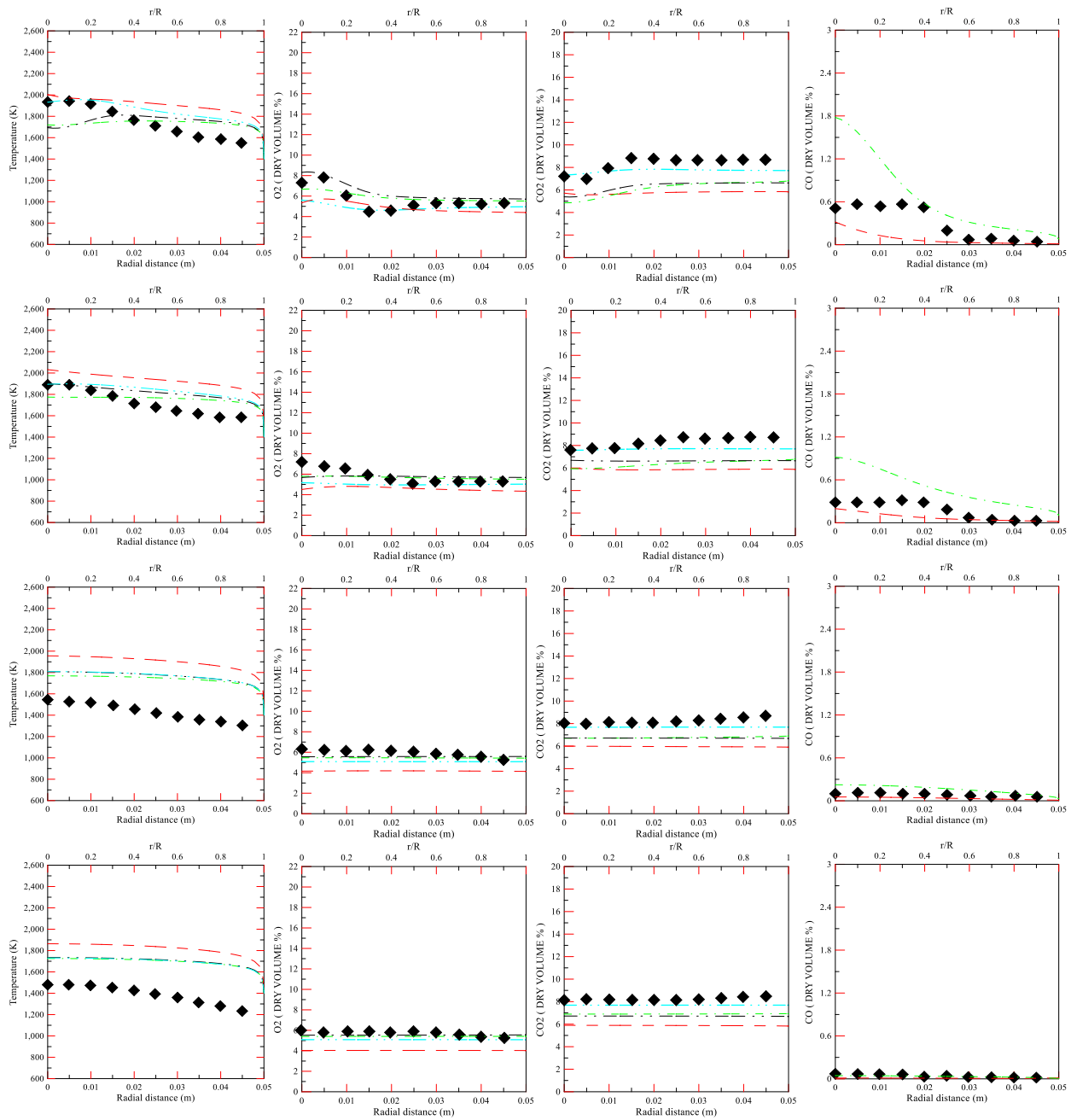


Figure 17 Predicted and measured radial profiles of mean temperature and dry volume fraction of CO₂ and O₂ at four axial locations (X/L = 0.432, 0.369, 0.510 and 0.632) respectively at different combustion modelling

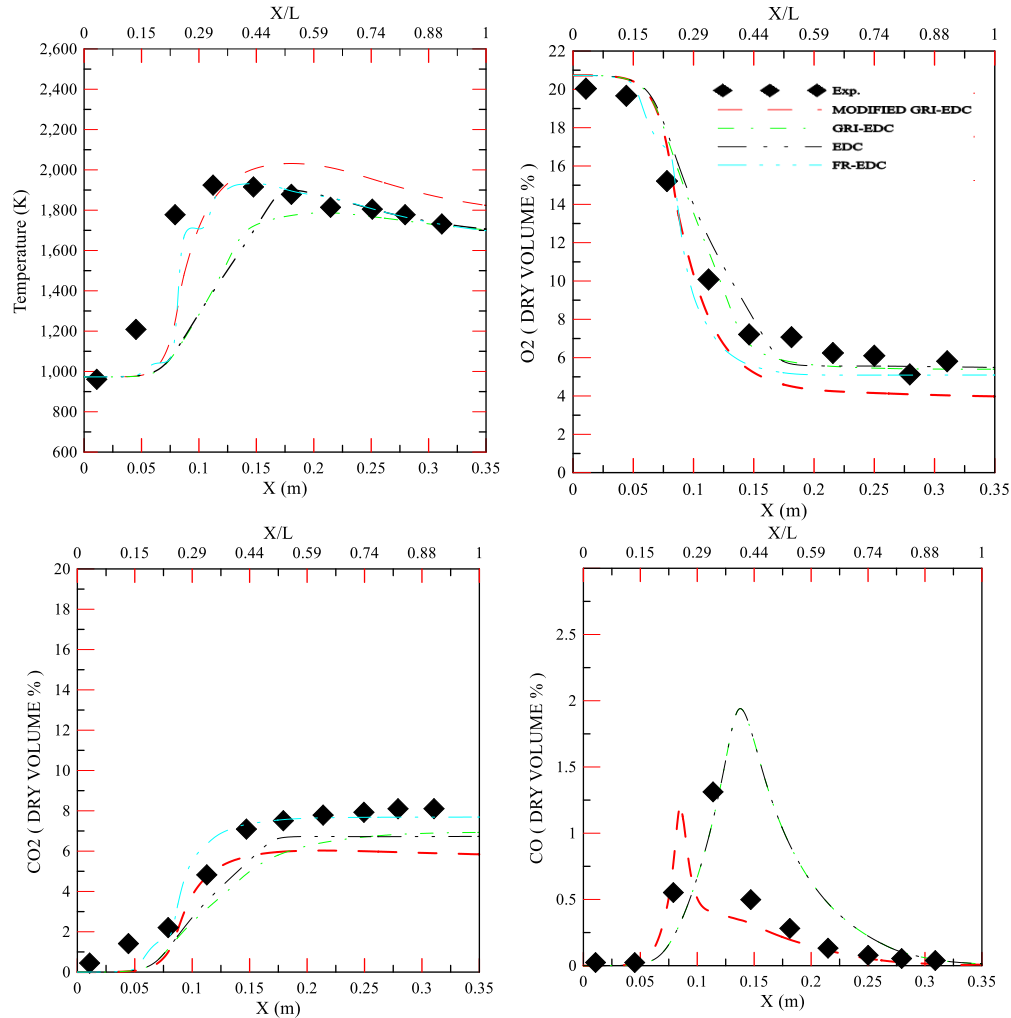


Figure 18 Predicted and measured axial profiles of mean temperature and dry volume fraction of CO₂ and O₂ at different combustion modelling.

5. Conclusions

In the present paper a computational investigation of flameless combustor was reported. Several turbulence models were compared with the experimental measurements of Verissimo et al. to evaluate the model performance., the following conclusions were drawn:

1. It was recommended to use realizable $k-\epsilon$ and RNG $k-\epsilon$ in flameless combustor modelling.
2. Taking radiation modelling in consider yields to a very small discrepancies for the predicted results therefore, it wasn't mandatory to take radiation effect in flameless modelling.
3. The performance of different combustion and reaction modelling were investigated. A deviation between predicted and measured temperature was noticed in all models, but EDC

and GRI-EDC yields to smallest deviation. A significant peak was observed in the predicted radial temperature measurements due to early ignition. This peak was controlled by changing values of volume fraction constant and time scale constant related to standard EDC model. In general, GRI-EDC was recommended to predict the mean temperature and dry volume fraction of O₂ and CO₂, but a relatively large deviation for predicted CO species.

6. References

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