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A Numerical Study on the Influence of CO_2 Dilution on Combustion Characteristics of a Turbulent Diffusion Flame

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***Abstract*—**The objective of the present study is to numerically investigate the effect of CO_2 replacement of N_2 in air stream on the flame characteristics of the CH_4 turbulent diffusion flame. The Open source Field Operation and Manipulation (OpenFOAM) has been used as the computational tool. In this regard, laminar flamelet and modified k-ε models have been utilized as combustion and turbulence models, respectively. Results reveal that the presence of CO_2 in air stream changes the flame shape and maximum flame temperature. Also, CO_2 dilution causes an increment in CO mass fraction.

***Keywords*—**CH_4 diffusion flame, CO_2 dilution, OpenFOAM, turbulent flame.

I. Introduction

THE global warming issue has become a major concern in recent years. Increasing the level of carbon dioxide, as a prominent contributor to global warming, and other pollutant emissions in the atmosphere leads to significant climate changes and can be detrimental for human health [1]. In this regard, using different strategies to reduce emission levels seems unavoidable. In practical applications, the addition of CO_2 as a diluent to fuel or oxidizer stream is commonly used to decrease flame temperature and achieve lower pollutant emissions [2], [3]. As CO_2 is a combustion product, it can be easily extracted from exhaust gas by condensing water vapor exists in the combustion products. CO_2 dilution has a significant impact on the flame structure, flammability limits, and pollutant emissions. Several researchers have investigated the effect of CO_2 dilution on flame characteristics.

Liu et al. [4] depicted that CO_2 addition affects the flame structure and soot formation through dilution, thermal and chemical effects. Park et al. [5] studied the effect of different diluents in methane-air counterflow diffusion flames and showed that thermal effect of CO_2 addition leads to the flame temperature reduction. Etere et al. [6] considered the effect of CO_2 dilution on the structure and pollutant emissions of methane-air turbulent diffusion flames. They found that, with the higher diluent concentrations in the fuel stream, visible flame length, flame temperature, and consequently soot and NOx emissions are reduced, but it leads to an increase in CO concentration. Zhuo et al. [7] conducted a numerical study on the impact of N_2, CO_2, and H_2O addition on combustion characteristics of syngas turbulent non-premixed jet flames. Their results indicated that CO_2 diluted flames have the largest reduction of flame temperature among other diluents. Also, they showed that the CO_2 addition shortens the flame size. Lock et al. [8] compared the impact of fuel stream with air stream dilution by CO_2 on the lift-off process of methane-air coflow flames. Wang et al. [9] performed a numerical investigation on the physical and chemical effects of CO_2 and H_2O additives in the methane diffusion flames. They focused on the thermal and chemical effects of theses diluents on the flame temperature and Emission Index of CO (EICO). Xu et al. [10] investigated the effect of H_2O and CO_2 diluted oxidizer on the structure and shape of coflow diffusion flames. They reported that the thermal and chemical effects of CO_2 replacement of N_2 in air would lead to the reduction of flame temperature. Gascoin et al. [11] considered the effect of CO_2 dilution on the flame temperature distribution. Furthermore, several researchers studied the effect of CO_2 dilution on flammability limits and some emissions such as NOx [12]-[14].

The objective of current computational research is mainly to investigate the effect of CO_2 addition to oxidizer stream on the flame length, temperature distribution, and CO concentration in a certain bluff-body stabilized methane swirling flame [21].

II. The OpenFOAM Framework

Open source Field Operation and Manipulation (OpenFOAM) is an open source CFD software package written in C++. It contains numerous solvers which are designed to solve complex fluid flows involving combustion, turbulence, and heat transfer. It also includes tools for meshing and utilities for post-processing and data manipulation. This package has been developed by OpenCFD Ltd. at ESI Group and distributed by the OpenFOAM Foundation [16].

III. Combustion Model

In this research, the steady laminar flamelet model (SLFM) implemented in OpenFOAM has been used as combustion model [22]. SLFM is based on the assumption that the turbulent flames can be considered as an ensemble of small laminar diffusion flames named as flamelets, in which the chemical reaction zone is thin enough compared to the turbulent length scales [17]. One of the most important

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advantages of the flamelet model is that the flamelets calculation is independent of turbulent flow in the pre-processing step. In pre-processing step, flamelets are stored in a flamelet library. After that, thermodynamic properties and species mass fractions can be extracted from these tables using parameters such as mixture fraction (Z), its variance (Z″) and scalar dissipation rate (χ), transported in the turbulent code. The conservation equations of species mass fraction and temperature in the mixture fraction space can be written as:

$$\rho\frac{\partial y_k}{\partial t}-\frac{1}{2}\rho\chi\frac{\partial^2 y_k}{\partial z^2}-\omega_{\dot{k}}=0 \quad (1)$$

$$\rho\frac{\partial T}{\partial t}-\frac{1}{2}\rho\chi\left(\frac{\partial^2 T}{\partial z^2}+\frac{1}{c_p}\frac{\partial c_p}{\partial Z}\frac{\partial T}{\partial Z}\right)+\frac{1}{c_p}\sum_{k=1}^{n}h_k\omega_{\dot{k}}=0 \quad (2)$$

where ρ is the thermodynamic density, Y_k is the chemical species mass fraction, T denotes the temperature, c_p and h_k are the specific isobaric heat capacity and the specific enthalpy of species k, respectively. The chemical species source term which is marked by $\omega_{\dot{k}}$ can be calculated with the chemistry reaction mechanism. The scalar dissipation rate, χ, is regarded as an inverse diffusion time scale.

$$\chi=2D\left(\frac{\partial Z}{\partial y}\right)^2 \quad (3)$$

χ is the function of mixture fraction and can be parameterized by its value at stoichiometric mixture, χ_{st}. In the current study, the flamelets are computed via the open-source chemistry software Cantera in which the scalar dissipation rate is adjusted by changing mass flow at fuel and oxidizer inlets.

Then, the mean value for species mass fraction and temperature are calculated by using Favre Presumed Probability Density Function (PDF).

$$\widetilde{Y_k}=\int_0^\infty\int_0^1 Y_k(Z,\chi_{st})P(Z,\chi_{st})\,\partial Z\,\partial\chi_{st} \quad (4)$$

$$\widetilde{T_k}=\int_0^\infty\int_0^1 T(Z,\chi_{st})P(Z,\chi_{st})\,\partial Z\,\partial\chi_{st} \quad (5)$$

Two additional transport equations for the mean mixture fraction and its variance have to be solved.

$$\frac{\partial\bar{\rho}\tilde{Z}}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_i\tilde{Z}}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\mu_{eff}\frac{\partial\tilde{Z}}{\partial x_i}\right) \quad (6)$$

$$\frac{\partial\bar{\rho}\,\partial\widetilde{Z''^2}}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_i\partial\widetilde{Z''^2}}{\partial x_i}=\frac{\partial}{\partial x_i}(\mu_{eff}\frac{\partial\widetilde{Z''^2}}{\partial x_i})+2\mu_{eff}\left(\frac{\partial\tilde{Z}}{\partial x_i}\right)^2-\bar{\rho}\tilde{\chi} \quad (7)$$

Here, the effective viscosity is consisted of a laminar and a turbulent contribution ($\mu_{eff}=\mu+\mu_t$) in which the eddy viscosity (μ_t) can be calculated by using a turbulence model.

The mean scalar dissipation rate in the mixture fraction variance equation can be modeled as:

$$\tilde{\chi}=C_\chi\frac{\varepsilon}{k}\widetilde{Z''} \quad (8)$$

$C_\chi=2$. Also here, k and $\mathcal{E}$ are the turbulent kinetic energy and its dissipation respectively. In this study, the chemical reaction mechanism applied for the CH_4 combustion is GRI 2.11 with 49 species and 277 reactions [18].

IV. Modified K-Epsilon Turbulence Model

Among the several turbulence models which have been employed for simulation of the bluff-body swirl flames, the modified k-epsilon model (by changing the constant $C\varepsilon_1$ from 1.44 to 1.6) has been proposed to improve the prediction of flow field and compensate for excessive diffusion [19], [20].

V. Numerical Modeling

The experimental data obtained by Al-Abdeli and Masri [21] was used for validation purpose. The schematic of burner is depicted in Fig. 1. The swirl burner is located in wind tunnel with about 2% free stream turbulence and the area of 130 mm square.

The 60 mm-diameter swirling annulus which provides the flow of pure air encompasses the stream of a fuel jet and a ceramic bluff-body face. In the other words, fuel and oxidizer are separated by a bluff-body which generates recirculation zones in the flow field [23]. The diameter of the fuel jet and the bluff-body face is 3.6 and D=50 mm, respectively.

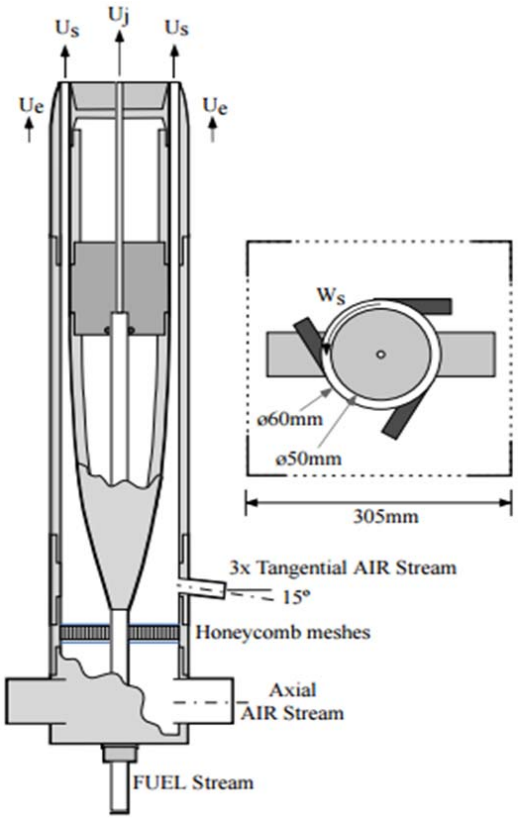

Fig. 1 The schematic of burner [24]

The boundary condition and flow properties of the reacting field such as the fuel jet velocity (U_j), the axial annular velocity (U_s), the tangential annular velocity (W_s), and the

velocity of co-flow air stream in the wind tunnel (U_e) are listed in Table I.

In the current research, the swirl number is set to be W_s/U_s=0.5. Also, the Reynolds numbers of fuel jet and swirl air flow are considered to be 7200 and 75900, respectively.

TABLE I
FLOW PROPERTIES

case	Fuel	oxidizer	U_j (m/s)	U_s (m/s)	W_s (m/s)	U_e (m/s)
Swirl flame	Methane	air	32.7	38.2	19.1	20

A 2-D wedge-type computational domain which is discretized into 45000 cells (180 and 250 cells in radial and axial directions respectively) has been considered in this simulation. To obtain a better accuracy, a mesh structure with higher resolution close to the wall and inlet boundaries are defined.

Fig. 2 shows the configuration of 2-D wedge-type grid. The flow field should be fully-developed at the exit plane. For this reason, the inlet flow streams are extended upstream of the exit plane to D=50 mm. In the current research, the OpenFOAM has been used as the computational toolbox. The code solves Favre-averaged Navier-Stokes and continuity equations. The Reynolds stresses are closed using modified *k*-epsilon model. The PISO algorithm is utilized for pressure-velocity coupling.

A Dirichlet condition is applied in the inlet for the velocity and mixture fraction fields, and a Neumann condition is set in the outlet boundary. Also, the pressure is fixed in the outlet and side boundaries, while a Neumann condition is applied for the inflow.

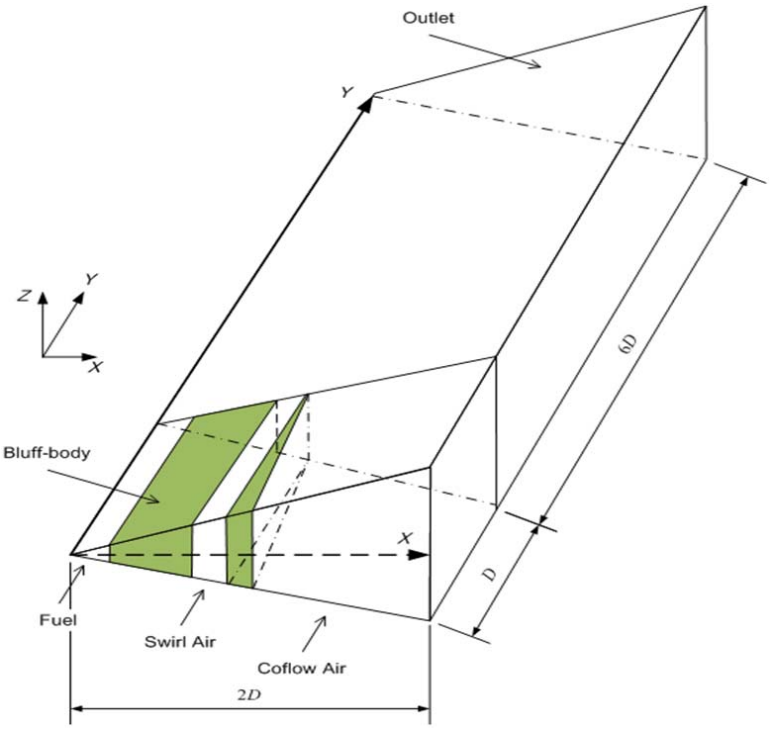

Fig. 2 The configuration of 2-D wedge-type computational domain

VI. Results and Discussion

A. Grid Dependency

The grid independency study has been done by changing the number of cells from 15000 to 75000 considering a mesh structure with higher resolution in the regions with high gradient of swirl velocity. This is because the most deviation from experimental data has been observed in the regions with higher velocity gradients. In Fig. 3, the effects of three different grids on the velocity and temperature profiles have been investigated in certain axial locations.

Although the grid with 15000 cells is unable to predict the aforementioned profiles properly, the difference between the simulation results of 45000 and 75000 cells is negligible, and no significant changes are observed in the simulation results. Consequently, the grid with 45000 cells has been utilized in this study.

B. Validation

Simulation results are compared with experimental data and previous studies [15] for temperature, axial and circumferential velocity components, and these results are depicted in Figs. 4-6. This comparison reveals that the predicted results are in a good agreement with the measurements and the general trend of profiles can be captured with an acceptable accuracy. It is worth mentioning that a similar level of accuracy has already been reported regarding the simulation of this swirl flame in previous related

studies [15]. Fig. 4 compares the calculated axial velocity component with measurements in different axial locations. It shows some inaccurate predictions around the centerline. This can be explained considering the low capability of RANS models regarding the simulation of shear flows.

C. Effect of CO_2 Addition to the Air Stream

The main objective of this research is the study of CO_2 addition to the air stream and its effect on the flame length, flame temperature distribution and CO mass fraction. To achieve this aim, different amounts of CO_2 are added to the air. The velocity boundary condition and the jet nozzle diameter kept unchanged and consequently, the mass flow rate of the air stream increases by CO_2 addition.

There are different definitions for the non-premixed turbulent flame length (L). The first one is that it can be determined based on the visible flame length. The second definition is that the flame length would be the axial location of peak temperature on the centerline. Also, the third definition states that flame length is considered as axial distance in which the mixture fraction would be stoichiometric on the centerline.

Since the studied flame structure in the present research has an hourglass shape, the farthest stoichiometric mixture fraction point is not always on the centerline. In this regard, the flame length is defined as the largest vertical distance between the nozzle exit plane and the stoichiometric mixture fraction point [15].

The details of different CO_2 dilution cases are depicted in Table II. The flame length is decreased slightly with the addition of CO_2. Actually, by CO_2 replacement of N_2 (i.e. by addition of CO_2), the density of oxidizer is increased and this could lead to increment of the oxidizer momentum. The slight increase in the momentum of oxidizer flow may result in production of stronger recirculation zones in the flow field which can increase the degree of mixing. This increment in mixing may lead to the reduction of flame length.

TABLE II
THE PERCENTAGE OF DILUTION AND CORRESPONDING DATA IN DIFFERENT CASES

Case	oxidizer Composition	Z_{st}	L/D
Case 1	10%CO_2+69%N_2+21%O_2	0.0528	2.060
Case 2	15%CO_2+64%N_2+21%O_2	0.0512	2.032
Case 3	20%CO_2+59%N_2+21%O_2	0.0498	2.016

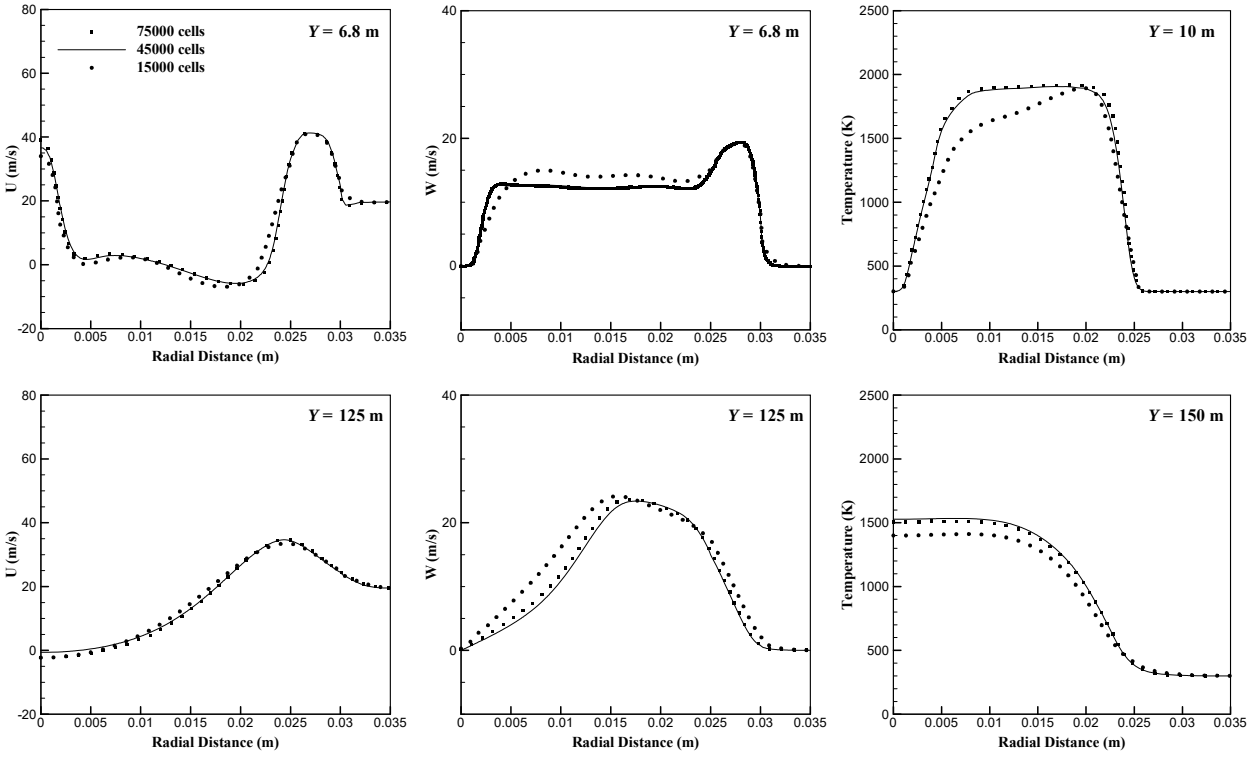

Fig. 3 Grid resolution study for radial profile of predicted temperature and velocity components at different axial locations using three mesh structure with 15000, 45000, and 75000 cells

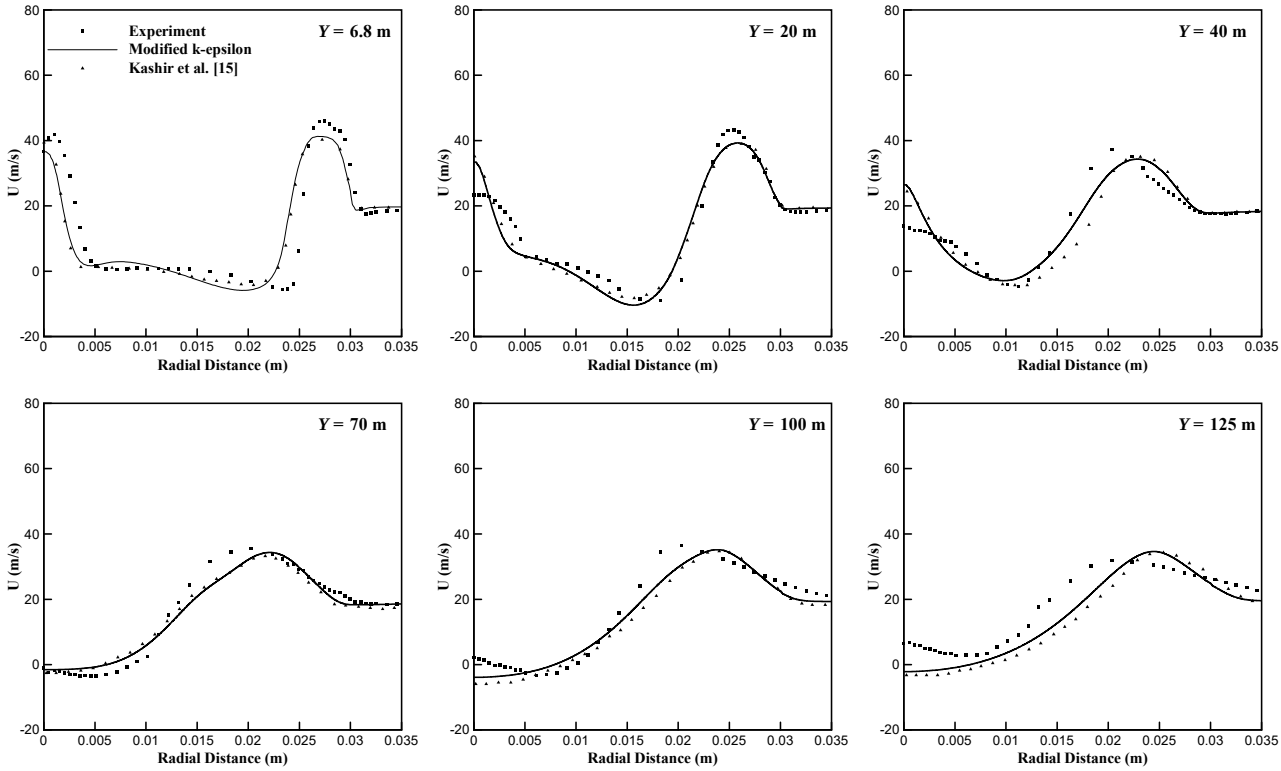

Fig. 4 Radial profile of predicted axial velocity component compared with measurements at different axial locations

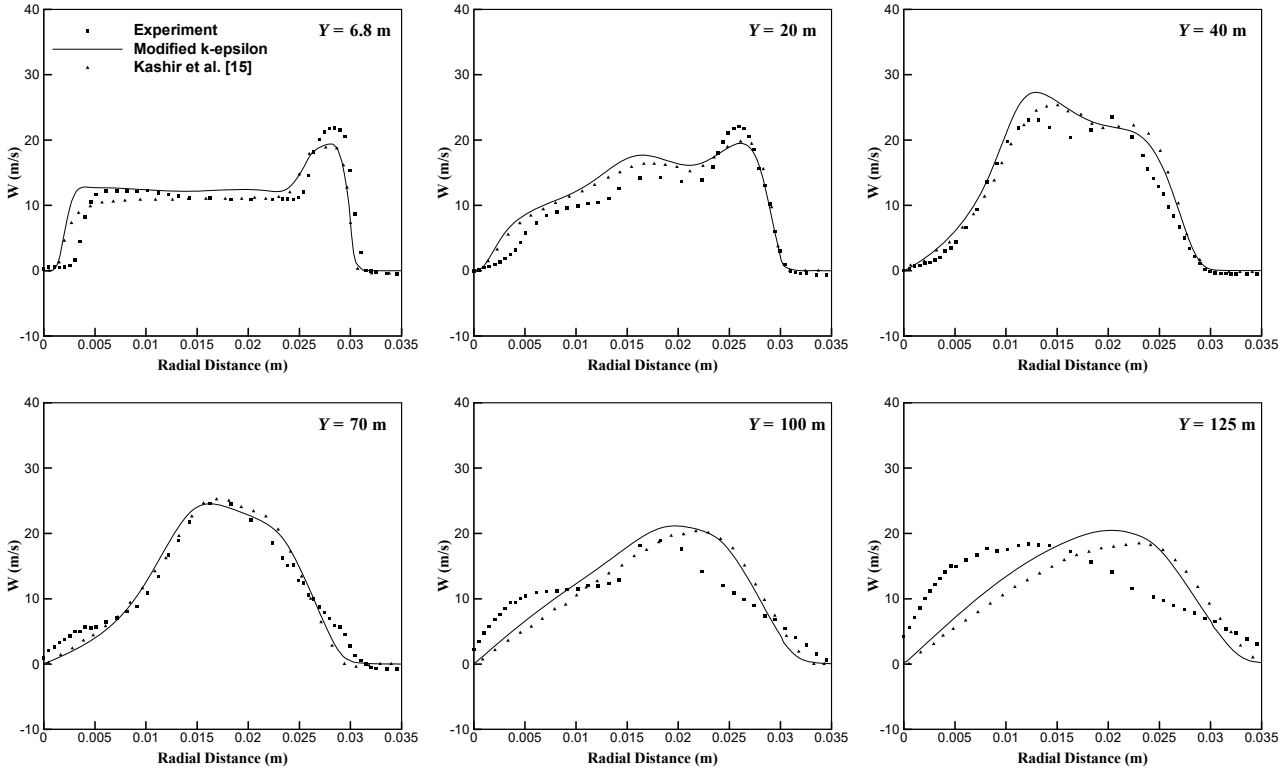

Fig. 5 Radial profile of predicted circumferential velocity component compared with measurements at different axial locations

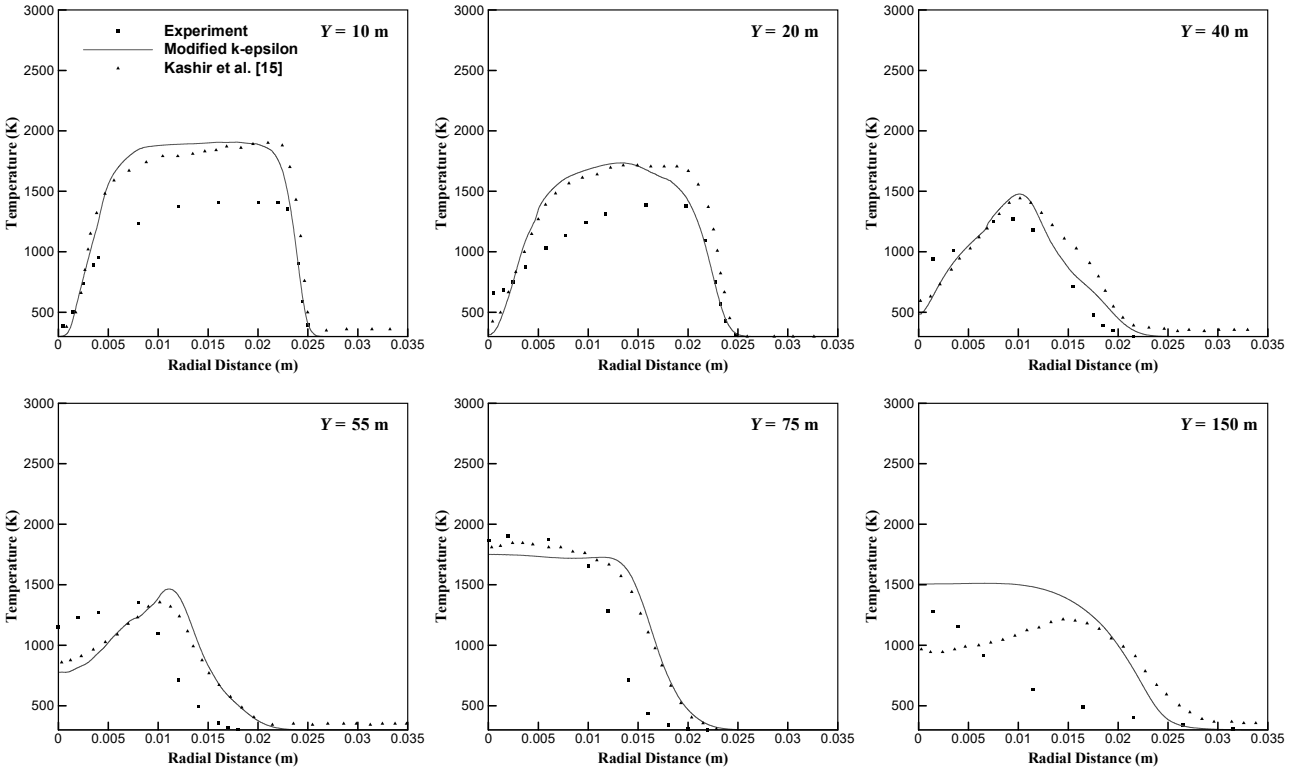

Fig. 6 Radial profile of predicted temperature compared with measurements at different axial locations

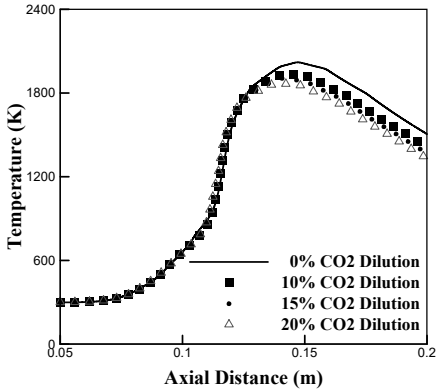

Fig. 7 Effect of CO_2 dilution on the flame temperature distribution along the centerline of nozzle

The effect of CO_2 addition instead of N_2 on the flame temperature distribution along the centerline is depicted in Fig. 7. This figure indicates that the temperature decreases by addition of CO_2. It is worth mentioning that, compared with the case of no CO_2 dilution, the peak temperature in Fig. 7 reduces around 83, 117, and 151 K by adding the amount of 10%, 15% and 20% of CO_2, respectively.

This can be explained by the higher heat capacity of CO_2 compared with N_2 which can lead to the reduction of flame temperature [10], [11], [14]. It is also interesting that the maximum flame temperature on the centerline (which can be assumed as a measure of flame length) moves toward the upstream of flow.

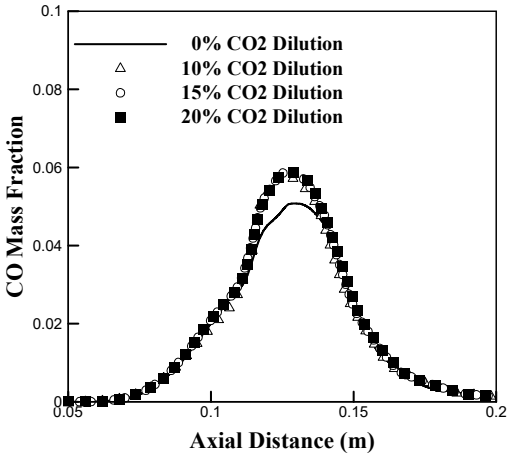

Fig. 8 Effect of CO_2 dilution on the CO Mass Fraction distribution along the centerline of nozzle

Fig. 8 shows the radial profile of CO mass fraction distribution on the centerline of flow field. This figure demonstrates that increase of CO_2 (compared with the case of no CO_2 dilution) leads to the increment of CO mass fraction in a certain region along the centerline. It is also interesting that, based on the calculations, a recirculation zone is created in the same region. This increase of CO mass fraction with addition of CO_2 might be due to the reduction of temperature in this

region (please see Fig 7).

VII. Conclusion

The effect of CO_2 replacement of N_2 on the characteristics of a turbulent diffusion flame was studied numerically. The OpenFOAM platform has been utilized as the computational tool. At the first stage, the simulation results were compared with reported experimental data and previous related studies. The comparisons revealed that predicted results were in good agreement with the measurements and simulations were able to capture the general trend of temperature and velocity component profiles with an acceptable accuracy. After the validation process, the effect of CO_2 addition to air stream was investigated. Results showed that the flame length and the maximum flame temperature were reduced by addition of CO_2. Furthermore, CO_2 dilution led to the increase of CO mass fraction.

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