Computational study of small-scale laminar coflow diffusion flames: influences of fuel dilution on the negative buoyant flame

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Abstract. The effects of adding H_2O and CO_2 on the hydrodynamic structure of laminar diffusion hydrocarbon flame was investigated at atmospheric pressure, focusing on the recirculation zone in the vicinity of nozzle exit with buoyancy force applied to the fuel. H_2O and CO_2 diluent were used to dilute the propane fuel focusing on how these diluents affect the vortices inside the recirculation zones. To clarify the influence of diluents, H_2O and CO_2 content (in mole basis %) in the fuel mixture was gradually increased from 0 to 20%. The numerical computations were performed using one-step gas-phase chemistry, thermal, and transport properties. The computational results of non-diluent propane fuel found to be in good agreement with available experimental data. The results showed that the fuel dilution notably influences the flow-field. In particular, the dilution of fuel with H_2O and CO_2 weakens the vortices formation. With increasing the diluents ratio, the scale of vortices structure becomes smaller. The results also showed that H_2O -diluent was more effective in reducing the vortex scale compared with CO_2-diluent.

1. Introduction

Diffusion flame exists in most practical combustion devices, and an accurate understanding of their structure is essential in the development of various combustion systems. The need to study a very simple geometric configuration is well fulfilled in the configuration of co-flow diffusion flame, where interactions between fluid dynamics, heat transfer and chemical reactions can be controlled and studied easily [1]. Therefore, co-flow diffusion flame is considered as the most frequently used. In addition, it provides a basic understanding of turbulent diffusion flames [2] and, easier to validate. Therefore, it is commonly used to improve the combustion models and characteristics such as gas-phase reaction [3], radiation [4], hydrodynamic structure [5], instability [6], polycyclic aromatic hydrocarbons (PAHs) [7,8] and soot [9,10].

It is a known fact that The formation of soot particles enhanced by flame flickering motions [11,12], Flame flickering motions are closely associated with the buoyancy-induced vortices near nozzle exit region [13,14], whereas these motions occur by accelerating the velocity of flow-field due to the buoyancy force [15,16]. Furthermore, buoyancy force distorted the parabolic velocity profile at an exit of fuel nozzle [13]. The relation of soot with the recirculation zone has also been addressed by many studies, Mueller et al. [17] conducted an experimental and computational study in turbulent non-

premixed bluff body flame, and they showed that the dynamics of the recirculation generate long residence time which supports surface growth, resulting in further soot growth.
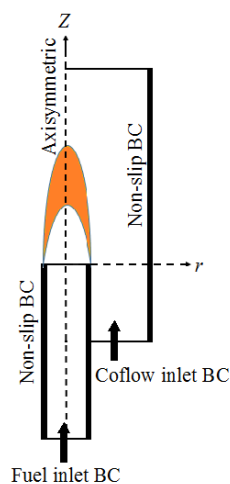
Large-scale vortex structure was observed in both turbulent and laminar diffusion flame, according to the experimental study [18] which identified two of vortices structures: the first one observed on the oxidizer side close to the flame bulge, and the second inner vortex is due to shear layer instability. Furthermore, the toroidal vortex which identified at the end of a potential core, this vortex identified in heavy fuel when the coflow air velocity was lighter than that of the fuel jet [13,19,20]. The experimental study of propane jets with lifted flames reported that the flow-field in the vicinity of the nozzle could significantly influence when notable difference in density existed between air and fuel [21]. Recently in the experimental study of small laminar coflow diffusion flame [22] with different types of hydrocarbon fuels methane, ethylene, propane, and n-butane, This study shows that a new recirculation zones were observed near the exit of fuel nozzle exit with fuels notably heavier than coflow-air (propane and n-butane).

Dilute the fuel stream with the combustion products technology have been developed to lower flame temperatures and reduce both soot and NO_x formation [23,24]. Since H_2O and CO_2 are a major component of combustion products, they are most frequently used as a fuel diluent. It is fundamental and practical importance to understand how the addition of H2O and CO2 to fuel affects the near-nozzle flow fields, in particular, on the formation of vortices near the fuel nozzle exit.

Given the above considerations, the purpose of the current study seeks to assess the influences of adding H2O and CO2 on the near-nozzle flow field in small-scale laminar coflow propane diffusion flames at atmospheric pressure, focusing on the recirculation zone in the vicinity of nozzle exit.

2. Numerical model and computational details

The computational study was performed for small-scale laminar coflow flames, ANSYS Fluent software package was used [25]. Two-dimensional non-uniform mesh was used covering a rectangular domain with a length of 110 mm and width of 30 mm. Mesh with 11800 computational cells with finest spacing in the regions directly above the fuel nozzle exit while coarser mesh points are used in the air coflow region to avoid expensive of computation time. Since the accuracy of simulation results may be sensitive to inlet boundary conditions [22,26], therefore the inlet boundary condition of fuel specified at Z_i= -70 mm far upstream of the nozzle exit by imposing a fully developed parabolic velocity profile, while a flat velocity profile was assumed for the coflow stream at Z_i= -10 mm. A schematic of computational domain and details of connected boundary conditions implemented in this study are shown in Figure 1.

Figure 1. Computational domain and connecting boundary conditions.
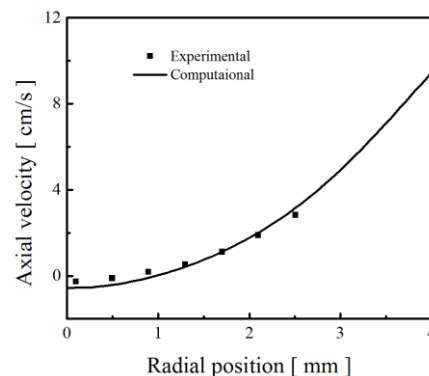
The governing equations for mass, momentum, energy, and species are solved in PISO pressure-velocity coupling fashion [27]. A second-order upwind scheme was adopted for spatial discretization.

One-step overall reaction is employed for propane [28]. The thermal and transport properties were taken from CHEMKIN III and TRANSPORT Package [29,30], respectively. The reference flame condition was specified as the same as that conducted by Xiong et al. [22] experimentally, such that the inlet temperature of the fuel and air was set as ambient temperature [298 K] with pure propane fuel. In fuel dilution set of simulations, the mole fraction of H_2O - and CO_2-diluents were set as 0.1 and 0.2. The mean velocity of propane fuel was set as 1.40 cm/s based on experimental condition [22], while the velocity of the air stream was set as 6.2 cm/s.

3. Results and Discussions:
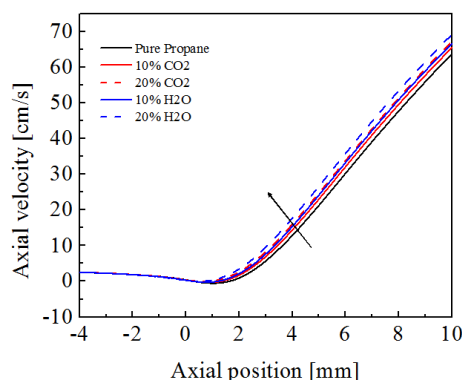
3.1 Validation of simulations:
Before discussing the effects of fuel diluents on the flow field, it is necessary to validate the simulation results with available experimental data. In this regard, the simulated radial velocity profile was compared with available experimental data in [22]. As presented in Fig.2 the predicted radial profile of axial velocity at height Z=1 mm above the nozzle exit for pure propane show excellent agreement with experimental data of Xiong et al. [22].
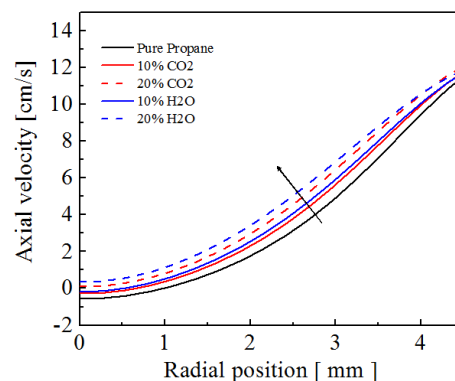

Figure 2. Comparisons of the radial profiles of axial velocity above nozzle exit at 1 mm; (symbols) experimental data of [22]; (solid line) current computational data.

3.2 Velocity Profiles
The predicted axial velocity profiles at centerline for propane with and without diluents are displayed in Figure 3. The predicted recirculation zone with negative axial velocity component appears in the near-nozzle region for around $0.45 < Z < 1.52$ mm with pure propane fuel, the negative component of the axial velocity decrease with added H_2O -or CO_2- diluent to the fuel stream. Dilution by either 10% H_2O or 10% CO_2 is effective to reduce the recirculation tendency.

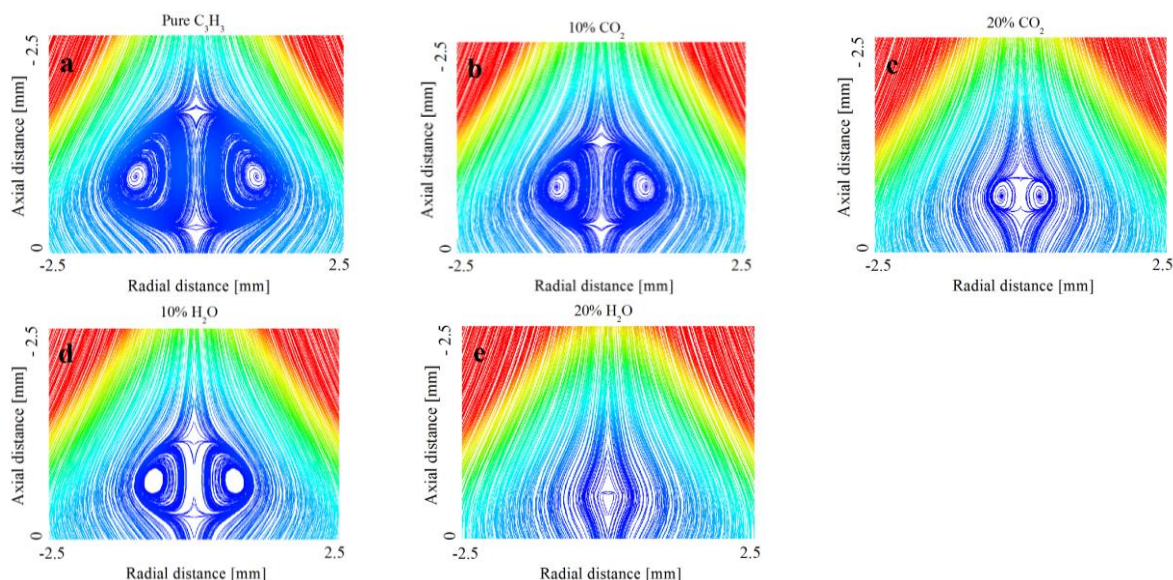**Figure 3.** Show axial velocity profiles along the centerline.

Figure 4. Show radial profiles of axial velocity at height Z=1mm.

As seen in Fig. 4 the axial velocity of the H_2O -diluted flame is slightly higher than that of the CO_2-diluted one. In addition, the region of negative axial velocity component diminish around $0.38 < Z$ 1.09 mm. with 20% of H_2O the negative component of axial velocity shift to the positive component for H_2O -diluted flame, while in 20% CO_2 it is limited to a small region just around $0.066 < Z < 0.076$ mm. The radial profiles of the axial velocity at height $Z = 1$ mm above the nozzle exit are shown in Figure 4, For pure propane, the axial velocity is below zero at the nozzle centerline, this is due to the propane fuel being heavier than air i.e., negative buoyancy. As the H_2O - and CO_2-diluent increased by 10%, the axial velocity at centreline increased about 51%. Again, the radial profile of axial velocity of the H_2O -diluted flame is higher than that of the CO_2-diluted one. For instance, the axial velocity of 20% H_2O - and 20% CO_2-diluted flame at centerline is 0.36 and 0.10 cm/s respectively, these results indicate that H_2O is more effective in increasing the axial velocity than CO_2-diluent. This may attribute to the faster diffusion properties of H_2O compared with CO_2.

3.3Effect of Fuel Dilution on Vortices
It is interesting to compare the results in the form of streamline between pure, H_2O - and CO_2 diluted flames as in Figure 6. With pure propane, two large-scale vortices structure can be identified near the exit of fuel nozzle as seen in Figure 5 (a), and that was found to be in satisfactory agreement with experiment [22].

Figure 5. Flow streamline visualization near nozzle exit for : (a) pure C_3H_8; (b) 10% CO_2 ; (c) 20% CO_2; (e) 10% H_2O ; (f) 20% H_2O.

It is speculated that these vortices are generated by the flow disturbance at the nozzle exit and amplified due to the appreciable difference in density between propane fuel and air [31]. With adding 10% H_2O and 10% CO_2-diluent to the fuel stream, the size of the vortices becomes smaller as seen in Figure 5(b) and (d) respectively, adding 10% of H_2O presents an even more significant reduction of the vortices size compared with 10% CO_2. As the H_2O increased to 20%, the vortices structure are dissipated as seen in Figure 5(e). While with 20% CO_2 the vortices structure still existed with small size. It is clear that the simulation result demonstrates the H_2O –diluent is more effective than CO_2-diluent. The changes in the density of the unburned fuel mixture (fuel and diluents) are the main responsible for the reduction of the vortices size near the nozzle. The differences in the results between the two diluent flames due to the differences in density between H_2O and CO_2-diluents. For example, the decrease in the fuel mixture density at nozzle exit for 20% CO_2 and 20% H_2O diluted

flame is 5.4% and 16.9% respectively. However, the CO_2 diluent effect has a smaller influence than H_2O when considering the higher density of CO_2 than H_2O.

4. Concluding remarks

We investigate computationally the effects of fuel dilution on the near-nozzle flow-fields focusing particularly on the vortices inside the recirculation zone in small-scale laminar buoyant coflow diffusion flames with propane fuel. The vortices scale inside recirculation zone decrease with increasing H_2O - or CO_2- diluent, the H_2O -diluent is more effective in reducing the vortex scale compared with CO_2-diluent. The diminishing of vortices scale is due to a significant decrease of the unburned fuel mixture density. Future work will focus on the dependence of sooting behavior on growth/decay of vortices inside the recirculation zone

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