A Comparison Between Water Addition and CO2 Addition to a Diffusion Jet Flame

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1   Abstract

This work compare the effects of adding water vapor and CO_2 to fuel for a diffusion flame. Water addition for the fuel side has demonstrated emission reduction, but whether the water molecules participate in the chemical and/or partial of the full process remains unknown. The objective of this research is to study the behavior of a methane diffusion flame with various amounts of water vapor and CO2 added to the fuel and to compare the flame behavior with various percentages of water vapor and CO2 content (0% to 65%). This work uses a coflow burner in PeleLM for simulating of the flame jet by computing the combustion behavior. The flame was simulated to pressures of 1.0, 1.4, 5.7, and 11.1 atm. The results extracted and analyzed include temperature profiles and various species mole fractions compared with their equilibrium state.

2   Motivation and Method

The current work research the effects of adding water vapor and CO_2 to fuel methane in a diffusion flame. Water and CO_2 are emissions from combustion processes, which can be recirculated and used, due to their low potential cost, to change flame properties [8]. Water addition has demonstrated its usefulness for NO_x emission reduction, peak temperature control, and fire suppression[9, 2, 1]. CO_2 addition has been shown to produce a change in flame peak, a reduction in soot formation, and flame height [4, 3]. The objective of this research is to study the behavior of a methane diffusion flame with various amounts of water vapor and CO_2 individually added to the fuel and to compare the flame behavior when the fuel is diluted with water vapor versus dilution with CO_2. Changing the diluent will help expose how much of the change is due to thermal properties of the diluent and how much can be attributed to changes in the flame chemistry. This work is entirely simulation-based but some relevant companion experiments have been published so that the simulation findings can be evaluated for reasonable trends.

The flame and combustion behavior is simulated in a coflow burner using a code called PeleLM. This code is developed by Lawrence Berkeley National Laboratory (LBNL) which uses an adaptive mesh refinement (AMR) for low Mach number reacting flows [7]. PeleLM allows the users to adjust the

refinement level of the mesh and the desired location on which the calculations are made and it utilizes the GRI 3.0 mechanism chemistry providing information on 53 species. While this is not the most comprehensive mechanism available for methane/air combustion, GRI 3.0 serves as an ideal baseline foundation for comparison because it is so widely used [5]. In addition, this mechanism has been shown to capture the key species and flame behaviors for coflow flames similar to those being studied in the current work. The simulation consists of a 64 x 256 coarse grid in a mesh of 10 x 40 mm in cylindrical coordinates. It is using a two-level refinement where the area of interest is the reaction zone of the flame. The boundary conditions consist of a slip wall (right side), flame axis symmetry (left side), inlet boundary (bottom side), and outflow (top side).

Table 1 shows the dilution and pressure conditions for the simulations done in PeleLM. Water and CO_2 mole fraction increase in increments of 10, except in the last case. Pressure conditions were at atmospheric conditions, 1.4 atm, 5.7 atm, and 11.1 atm. The pressure conditions were chosen to match experimental results at 1 atm, and the dilution conditions limited at the maximum to avoid flame extinction [6]. This work is primarily a large data set that spans three condition axes: diluent species, diluent fraction, and pressure. Hence, the results are mostly graphical to allow comparison between conditions and to expose situations where significant variations occur.

3   Results and Conclusion

The results extracted and analyzed include temperature profiles and various species mole fractions compared with their equilibrium state. Regarding physical properties both water and carbon dioxide present similar behaviors. At atmospheric pressure and high water content, the flame lifts off from the burner tip, while as the pressure rises the flame anchors back near the burner tip. In contrast, CO_2 addition does not lift the flame from the burner tip. As pressure rises, the flame width reduces. Both water and CO_2 addition decrease the flame peak temperature, as seen in Figures 1 and 2. Note that the aspect ratio of the figure images is not scaled but expands the horizontal axis to provide more visibility in the region near the burner exit. This artificial horizontal expansion highlights the narrowing of the flame with changes in pressure while much smaller change is visible with changes in diluent fraction. There is also relatively limited effect of diluent composition as the thermal images of flames diluted with water and carbon dioxide are very similar under similar pressure and dilution conditions.

In order to provide more structure details, Figures 3 and 4 show the mole fraction of oxygen, water, carbon dioxide, and carbon monoxide in the different conditions of the flames. In both cases, the temperature profile follows the same path as water and carbon dioxide respectively. The maximum mole concentration of CO_2 and CO were also investigated for all conditions. For the water addition, the CO_2 and CO have an increase of maximum concentration when pressure rises. From 1 to 1.4 atm, there is a decrease in the maximum concentration of CO. As for the CO_2 addition, there is an increase of CO in all conditions. H_2O and CO_2 concentration profile was also compared for all the conditions along the centerline of the diffusion flame. The rise of pressure produces an increase of water concentration approximately 0.4-0.6 mm from the burner, and it is observed that the water concentration decays slower than at lower pressure conditions. The addition of water and carbon dioxide has similar results on the flame behavior. Future work will include an analysis of existing high-pressure experiment results and the superequilibrium prediction for the species (H and O) at different pressures.

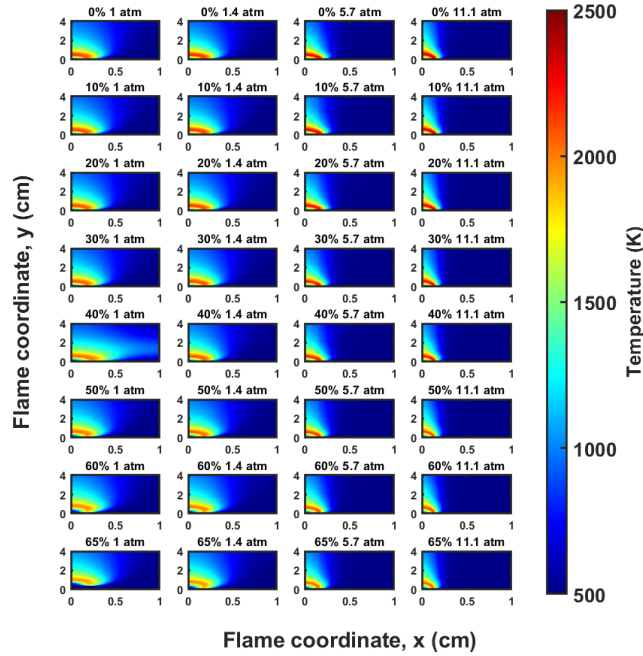## 4   Acknowledgment

5 Figures and Tables

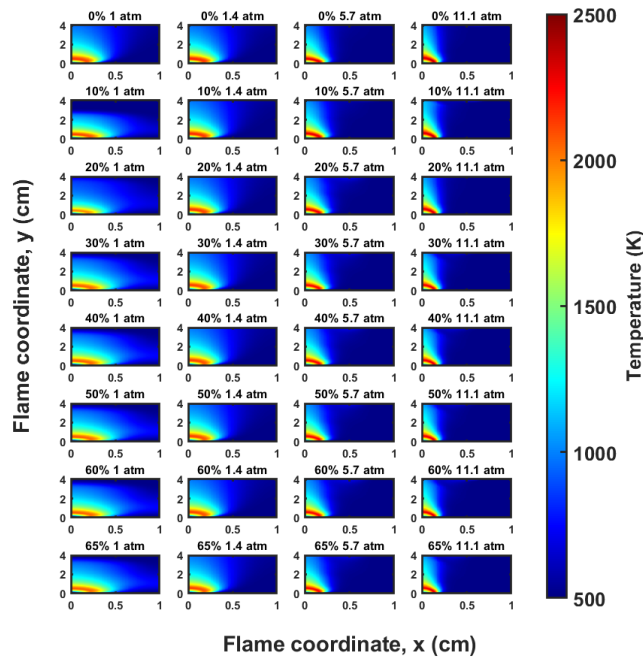Figure 1: H_2O Temperature of all flames under different conditions.

Figure 2: CO_2 Temperature of all flames under different conditions.

Table 1: Detailed conditions of the simulations.

| Mole Fraction	H_2O Velocity (m/s)		CO_2 Velocity (m/s)		Pressure (atm)
	Fuel	Air	Fuel	Air	
0	0.40	0.46	0.40	0.46	1
	0.29	0.33	0.29	0.33	1.4
	0.07	0.08	0.07	0.08	5.7
	0.04	0.04	0.04	0.04	11.1
0.1	0.44	0.46	0.43	0.46	1
	0.32	0.33	0.31	0.33	1.4
	0.08	0.08	0.08	0.08	5.7
	0.04	0.04	0.04	0.04	11.1
0.2	0.50	0.46	0.48	0.46	1
	0.36	0.33	0.34	0.33	1.4
	0.09	0.08	0.08	0.08	5.7
	0.04	0.04	0.04	0.04	11.1
0.3	0.57	0.46	0.53	0.46	1
	0.41	0.33	0.38	0.33	1.4
	0.10	0.08	0.09	0.08	5.7
	0.05	0.04	0.05	0.04	11.1
0.4	0.67	0.46	0.61	0.46	1
	0.48	0.33	0.43	0.33	1.4
	0.12	0.08	0.11	0.08	5.7
	0.06	0.04	0.05	0.04	11.1
0.5	0.80	0.46	0.71	0.46	1
	0.57	0.33	0.51	0.33	1.4
	0.14	0.08	0.13	0.08	5.7
	0.07	0.04	0.06	0.04	11.1
0.6	1.00	0.46	0.87	0.46	1
	0.71	0.33	0.62	0.33	1.4
	0.18	0.08	0.15	0.08	5.7
	0.09	0.04	0.08	0.04	11.1
0.65	1.14	0.46	0.98	0.46	1
	0.81	0.33	0.70	0.33	1.4
	0.20	0.08	0.17	0.08	5.7
	0.10	0.04	0.09	0.04	11.1
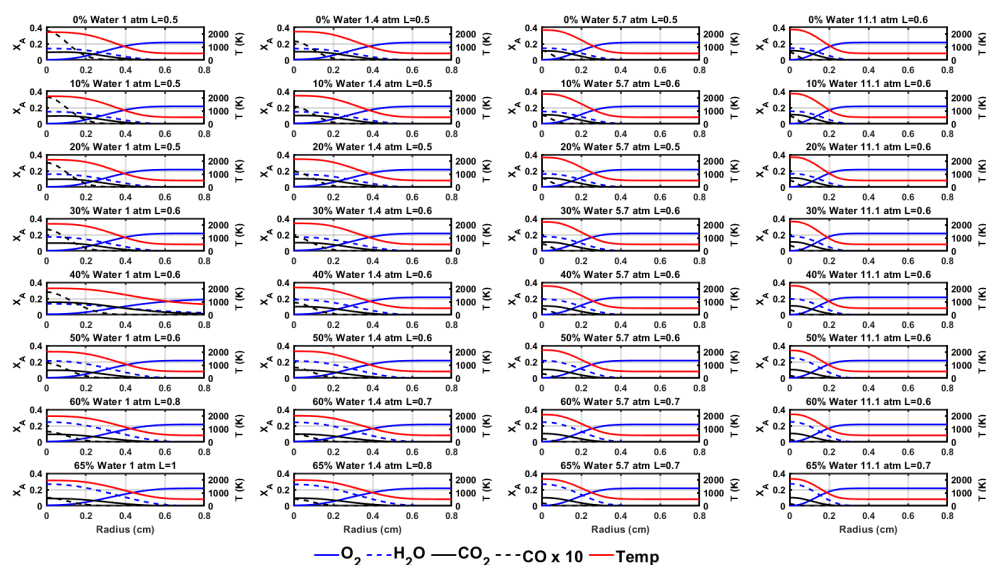
Figure 3: H_2O Temperature and species mole fraction along the flame radius. CO concentration is x10 for all of the conditions.
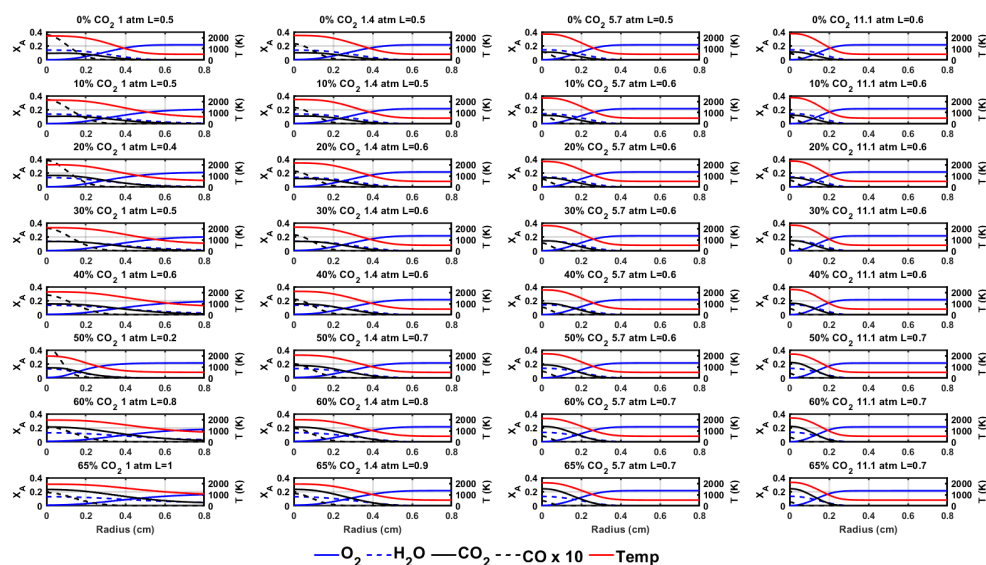

Figure 4: CO_2 Temperature and species mole fraction along the flame radius. CO concentration is x10 for all of the conditions.

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