CFD Modeling of pressurized laminar coflow (non-premixed) diffusion flames with water addition

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1 Introduction

This research aims to examine the effect of water vapor addition to pressurized flames by computation. It is a continuation of a series of experiments and numerical simulations focused on the addition of very high levels of water vapor to the fuel side of diffusion flames. The prior sequence of studies includes methane hydrate flames, counterflow diffusion flames, coflow diffusion flames at 1 atm, and coflow diffusion flames at high pressure but without water addition. All of these prior works, and the current one, are motivated by the continuing uncertainty regarding the role of water as a diluent.

It has been shown in prior studies [1-2-3] that using water dilution on flames is beneficial for fire suppression and that it decreases soot and NOx emissions. The science of whether if water vapor added to the fuel affects the chemistry, the thermal behavior remains questioning and is the goal of this work. A novel example for watery fuel combustion is methane hydrates burning from the deep ocean.

Vicariotto, et al. [4-5] studied the chemical and thermal effect of water addition to a laminar coflow diffusion flame. The result shows that steam water was not a non-reactive inert diluent but could be an active reactant in the combustion process. The studied is focused on the effect of water addition on OH production in the flame maintaining either a constant methane flow rate or total mass flow rate.

Escofet-Martin et al. [6-7] experimented the very similar coflow laminar diffusion flame with elevated pressure from 1 to 11.1 atmosphere, and addressed that the behavior of the flame, reaction kinetics and density are influenced by the ambient conditions. It is beneficial to study if water diluted flames have a change in behavior for instance, when subjected to various pressures.

The objective of the current work is to extend the prior research and study the effect of water addition to the fuel side of a laminar coflow diffusion flame under different pressures, and identifying whether water addition changes or not chemical reactions. This study relies on the use of the CFD code PeleLM [8]. PeleLM is an open-source adaptive-mesh low Mach number hydrodynamics code for reacting flows. GRI-Mech 3.0 [9] mechanism is used to model the natural gas combustion.

2 Simulations

The numerical simulation burner geometry is based on experimental setup [4-7]. The flame is established on a co-annular burner. The physical experiment is a small extruded tube for fuel flow and

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coannular pipe for the oxidizer (air) flow. The details of the burner diameters will be addressed in the following paragraphs together with the computational domain.

While the PeleLM code has not implemented the extruded geometry yet, this study is modeled using the flush geometry. This means that the air, the fuel and the oxidizer enter the computational domain at the same vertical location at the same level of outlets. Previous research has shown that this can have an effect on the results particularly at low water concentrations. Moreover, with increasing the amount of water, the flame is lifted away from the burner exit which reduced this effect of the geometry configuration. In addition, the inlet flow of air has a hyperbolic tangent profile which can simulate the growth of a boundary layer along an extruded tube and so this further mitigates the difference between physical and computational geometry.

The fuel burner is 10-mm radius with a separate fuel/oxidizer outlet. The computation uses cylindrical coordinates assuming the burner and the flame are axisymmetric. Therefore, the computational domain is defined as a 10x40 mm rectangle and the initial condition fills the domain with air at 300K and the pressure condition under study.

Boundary conditions provide a set of constraints to resolve the differential equation for the computational domain. As shown in Figure 1, the z-axis on the left (yellow) represents the flow direction which is the center of the burner. The blue color on the right-hand side is an impermeable slip wall with adiabatic boundary, where the gradient of temperature is zero. The top boundary (grey bar) is set as outflow. Pressure in the whole domain is always constant and varies in this work among 1, 1.4, 5.7, and 11.1 atm. These pressure values are chosen to be consistent with the previous experimental works [6-7]. The bottom is the inlet boundary, where the values for inlet temperature and velocities are specified. The wall of the fuel tube is also shown in Figure 1 at radius 0.9 mm horizontal location (fuel_ox_split) meaning the burner edge. The fuel inlet velocity profile is set to parabolic, with the averaged velocity matching the constant methane flow rate (35 mL/min, 29.9 cm/s) of the experiments, and the inlet temperature is preheated at 510 K for water vaporization. The fuel region is then followed by a 0.2 mm zone (Vel_zero_th) where no gases enter the domain which represents the fuel tube wall and the extruded tube. The remaining of the bottom boundary, until Ox_air_split, is the oxidizer inlet. The air (oxidizer) inlet temperature is fixed at 510 K, and the air velocity is equal to the experimental velocity of 46 cm/s

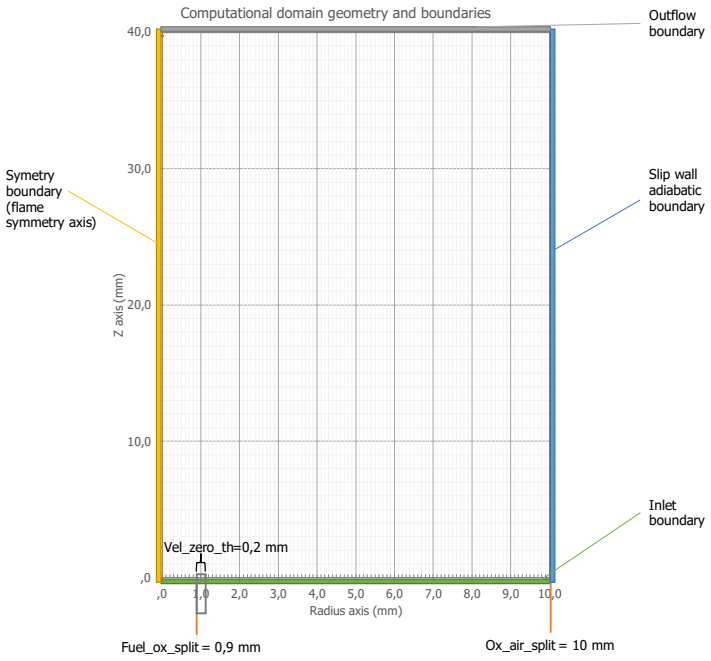

Figure 1: Computational domain geometry and boundary conditions.

(in ambient pressure), with a nearly top hat profile. The code actually uses a hyperbolic tangent velocity profile for the air stream to avoid any problem at the interface between the air and the fuel tube wall so the top hat is effectively rounded off near the fuel tube.
Finally, there are multiple zones defined in the computational domain as follows:

- At the Inlet boundary, from radius 0 to the fuel_ox_split, the zone is Fuelpipe zone.
- At the Inlet boundary, from fuel_ox_split to ox_air_split the zone is Oxidizer zone.
- At the Inlet boundary, the Air zone is after the ox_air_split.
- There is also an Outflow zone and a Volume zone (volume of the computational domain).

For all of the water dilution conditions in this study, methane flow rate is constant at 35 ml/min for matching the molar fraction (instead of mass fraction). The water dilution, hence, increases the total mass flow and the fuel inlet velocity. When the pressure of the ambient rises, the fuel and the oxidizer inlet velocities are decreased due to the density change.

The table 1 resume the cases treated during this study.

Table 1: Characteristics of the different CoFlow diffusion flame simulations.

H2O mole fraction, %	Pressure, atm	Inlet fuel Velocity, m/s	Inlet oxidizer Velocity, m/s
0	1	0.399	0.462
	1.4	0.285	0.330
	5.7	0.070	0.081
	11.1	0.0359	0.0416
10	1	0.443	0.462
	1.4	0.317	0.330
	5.7	0.078	0.081
	11.1	0.0399	0.0416
20	1	0.499	0.462
	1.4	0.356	0.330
	5.7	0.088	0.081
	11.1	0.0499	0.0416
40	1	0.665	0.462
	1.4	0.475	0.330
	5.7	0.117	0.081
	11.1	0.0599	0.0416
60	1	0.998	0.462
	1.4	0.7125	0.330
	5.7	0.175	0.081
	11.1	0.0899	0.0416

In this study, to determine the appropriate convergence of the code, the steady state is defined when the relative error of species mass fraction and major variables such as temperature, density, etc. between 100 time steps is below 0.5%. The relative error is shown in the following equation:

$$\epsilon_r = \frac{\|A_0 - A_{100}\|}{\|A_0\|},$$

Where A_{100} is the value of A_0 after 100 time steps.

PeleLM uses adaptive mesh refinement (AMR) to regrid the mesh, creating finer grids in the coarser grids until the solution is sufficiently resolved. The code also evaluates where additional refinement is needed according to user criteria. In current computational diffusion flame, a maximum of two levels of refinement above the coarse grid is used. In this research at the first level, the additional refinement is set near the high temperature gradient. The second level sets additional refinement near the nozzle in which OH concentrations are significantly distributed with high temperature gradient.

The results of the simulation are saved in a plot file every 100 time steps. There are tools equipped and available with the PeleLM code for converting plot files into for example, Matlab and Python data. Some visualization tools enable the user to print the profiles of simulated variables. The main tools used in this study are Amrvis, VisIt [10] and Matlab.

3 Results

Figure 2 shows the results of water addition to the methane at 0, 10, 20, 40 and 60% water addition. The maximum temperature of the flame decreases from 2137 K to 1984 K which is 7% reduction (from no water addition). Furthermore, the increased total flow of the fuel inlet velocity attributed in part to the water addition makes the flame taller. The case of 0.6 water mole fraction shown in figure 2 shows that the flame is lifted from the burner exit. A small increase in dilution between 0.6 water mole fractions to around 0.715 water mole fraction results in a more lifted flame until its extinction [4].

Figure 3 shows numerous temperature results (in kelvin) of simulated flame at 1, 1.4, 5.7 and 11.1 atm at 0%, 10% and 20% water mole addition. From left to right, the pressure raises from 1 atm to the maximum 11.1 atm. Note that 11.1 atm is near the maximum pressure of the limitations for the experiment before the flame starts flickering. Therefore, increasing pressure can lead to an unsteady flame.

There are two major effects observed from figure 3 as the pressure rises. One is that the flame maximum temperature is increased. The other is that the flame is stretched to be longer but thinner in the radial direction. This last effect is enhanced by water addition. As shown in figure 3 at the highest pressure (11.1atm), some fluctuations appear in the oxidizer zone. Those "vortices" may be responsible for the unstable flame. To further verify this hypothesis, the time history tracing the flow velocity in the coflow region is plotted, shown in figure 4. The result shows that the relatively high buoyant velocity interacts with the slow coflow velocity (at high pressure) to create an unstable shear layer. Furthermore, the fluctuations and "vortices" are due to the right-hand side slip wall boundary condition and consequently don't represent the reality. This effect is enhanced with water dilution. The number of time steps is needed to increase from 45,000 and beyond for achieving the better steady state results.

Further analysis on how water vapor addition effects or participates in the reaction particularly on hydroxyl and carbon monoxide is needed for understanding the influence from water addition and identifying the role of elevated pressures.

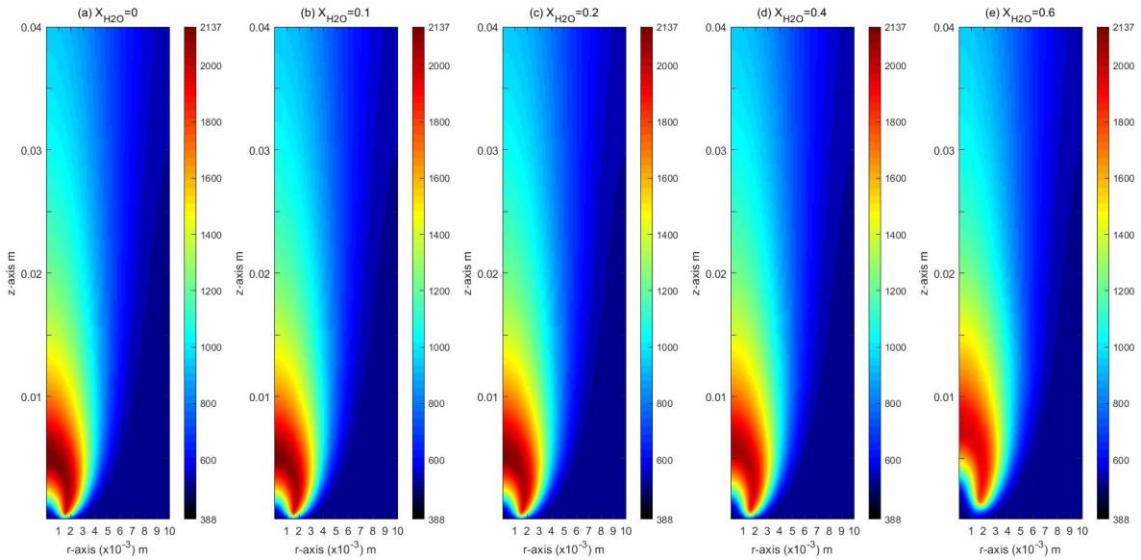

Figure 2: Simulated ambient pressure flame temperature (K) with water addition.

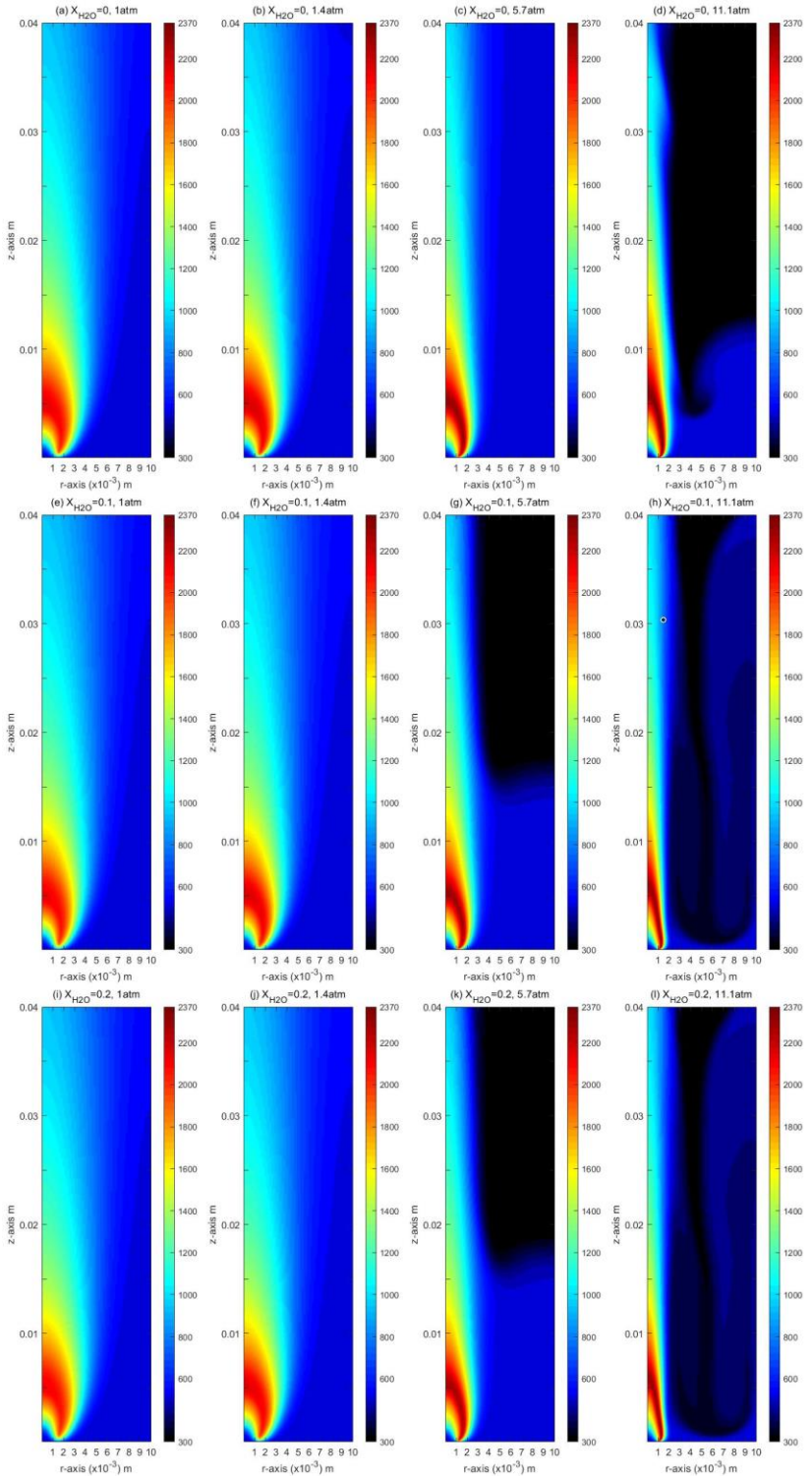

Figure 3: Simulated flame temperature (K) at 1, 1.4, 5.7, and 11.1 atm with 0%, (a) – (d), 10%, (e) - (h), and 20%, (i) – (l), water mole addition.

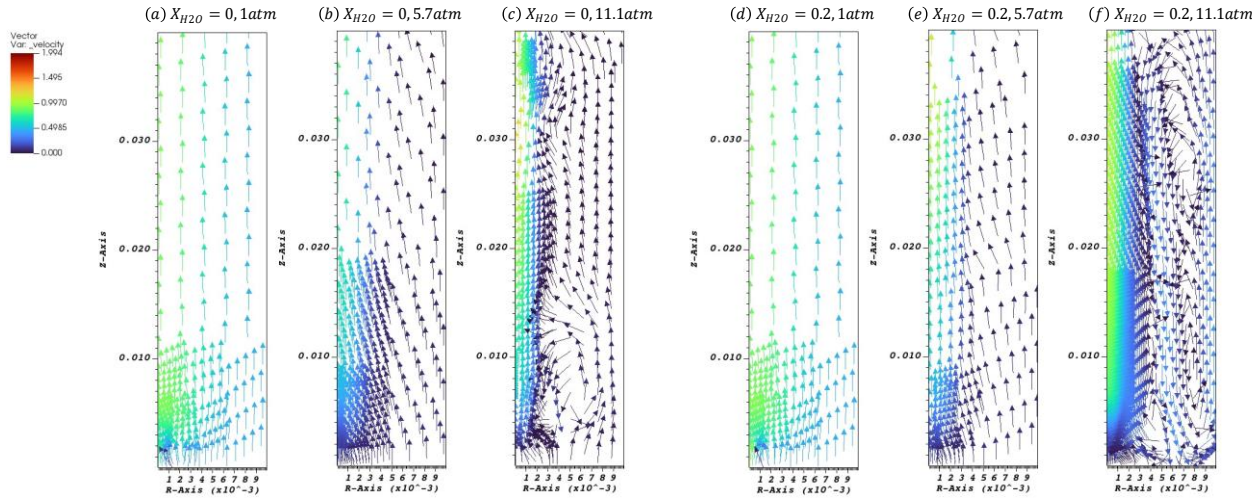

Figure 4: Simulated flame velocity profiles at 1, 5.7, and 11.1 atm with 0%, (a) – (c) and 20%, (d) - (f) water mole addition: The vector length only represents the direction.

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