Title
Numerical Simulation of Water-Vapor Addition into a Methane Diffusion Flame at High Pressures Using PeleLM

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Peer reviewed|Thesis/dissertation
NUMERICAL SIMULATION OF WATER-VAPOR ADDITION INTO A METHANE DIFFUSION FLAME AT HIGH PRESSURES USING PELELM

THESIS

submitted in partial satisfaction of the requirements
for the degree of

MASTER OF SCIENCE
in Civil and Environmental Engineering

by

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2021
DEDICATION

To the scientific and research community for their relentless effort towards the progress of mankind.
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This research explores the effects of adding water vapor to fuel for a diffusion flame. Inert gases have been used in the dilution of combustion commonly to reduce emissions. Water is a unique diluent because it provides important radical species influencing the flame, particularly with cooling or destabilizing effects when the enthalpy of the diluted fuel is reduced. The objective of this research is to study the behavior of a methane diffusion flame with various amounts of water vapor added to the fuel using a coflow burner and to compare the flame behavior with various percentages of water vapor added into the fuel. The present work continues previous studies on water-diluted flame behavior and explores the effect of elevated pressures. The simulation research uses PeleLM code for computing combustion behavior when water is added to diffusion flames. Besides various water content in atmospheric conditions, the flame was also simulated to pressures of 1.4, 5.7, and 11.1 atm. The results extracted and analyzed include temperature profiles and various species mole fractions such as CO₂, CO, OH, H, O, and H₂O. The overall flame images show that the flame base is lifted at higher water content conditions from the tip of the burner. At 0.65 mole water content and 11.1 atm, the flame base is observed anchoring back to the tip of the burner. When increasing the pressure, the flame, in general, becomes thinner and more compact, which means the reaction zone is reduced. The results show more drastic changes of flame
appearance at elevated pressures when beyond 5.7 atm, and the water addition into the
flame reduces the CO concentration. The computed H and O atoms are at superequilibrium
for about two to three times (more than the equilibrium) at lower pressure conditions and
around five times at higher water concentrations. OH remains near the equilibrium for all
the pressure and water conditions.
Chapter 1

Introduction

This chapter introduces the background perspective leading to the motivation of this research, addresses water addition combustion practices, and describes the research purpose of this thesis.

1.1 Background and motivation

Fossil fuels have been part of the development of our society, but with the increasing environmental and health awareness along with new legislation for particulate emission, there is a greater need than ever to reduce pollutants from practical combustion systems [2–5]. Greenhouse gases, which mainly consist of carbon dioxide (CO₂) and methane (CH₄), have accelerated global warming resulting in a series of adverse consequences to human beings, such as sea-level rise and a higher frequency of extreme weather [6].

As many countries are moving toward sustainable energy resources in the cities there are still large sectors that have difficulty reducing their carbon footprint. These sectors include, for example, the large class transportation, such as airplanes or large boats. Both of them
are currently reliable vehicles which generates useful power constantly from combustion [7]. These sectors cannot easily let go of carbon based fuels. Therefore, the study of combustion processes remain important. The importance of understanding mechanisms that might employ fuel dilution may help in achieving combustion efficiency and in the decrease of carbon footprint.

1.2 Practice of water-vapor laden fuel combustion

Additives in flames is one of the methods utilized to mitigate or control pollutant emissions from combustion processes. The additives have different consequences in combustion, and the most used are the burned product gases in what is called flue gas recirculation [8]. These gases such as argon, carbon dioxide, nitrogen have been used in the dilution of combustion. They are most commonly used to reduce emissions, and water is often identified as a unique diluent because it can provide important radical species to help offset the destabilizing effects of the reduced enthalpy of diluted fuel.

The addition of water has been taken as most relevant in past years as an approach to increase efficiency and reduce pollutants. The studies of water addition in the fuel and oxidizer streams investigated its effects in flame. This is relevant in applications like NO\textsubscript{x} reduction in gas turbine cogeneration systems [9], soot reduction, and fire suppression [10, 11]. During the burning of methane hydrate, there is a significant amount of water participating in the process [12–14].

The review by Dryer about water dilution describes the practical applications and fundamental concepts in combustion systems. For example, its physical effects and chemical effects in applications can improve fuel atomization, reduce NO\textsubscript{x} emissions in gas turbines, and provide peak temperature control. Dryer [15] concluded that more fundamental research is
required on the chemical and physical effects of water. Therefore, understanding the role of water in its observed behavior in different combustion processes at different conditions may help explain inconsistencies in its observed effects in various combustion applications [15], which are yet to be explained.

1.3 Objective

The current research continues the exploration of water-vapor laden fuel combustion, and extends from atmospheric pressure to high-pressure environments, where most practical combustors operate. There are several existing experimental and numerical studies with water addition, but they are usually conducted at atmospheric pressures and at low water addition (below 30% water content). This thesis will present not only the results from new numerical simulation, but will also reference the previous experimental and numerical studies in atmospheric pressure conditions as the foundation. The analysis involves the geometric change in physical appearance of the flame, flame temperature, and the concentration of various important species. The primary objective of this study is numerically identifying the behavior of a laminar methane diffusion flame when water is added to the fuel stream as the first step, and further understanding the key characteristics of this behavior, particularly under high pressure conditions.

The next chapters will cover a literature review for both water addition and high pressure combustion, a description of the numerical simulation, methods, followed by a discussion of the results and conclusion.
Chapter 2

Literature review

This chapter presents different studies about the addition of water as a diluent in methane laminar diffusion flames and the role of the molecules of water in combustion. Water addition under high pressure will also be included even though few studies have been made on this subject. This research is a continuation of previous work on water dilution in atmospheric conditions [1, 16], and an experimental study for high pressure combustion [17, 18]. A methane coflow diffusion flame was studied, where water was added to the fuel stream [1]. The current work is entirely numerical and includes both water addition and the effects of high pressure. The work relies on these prior studies as baseline particularly on the experimental results on coflow flames to further simulate the conditions at high pressure and with water addition. This chapter addresses the relevant studies on diffusion flames.

2.1 Burner

There are several types of burners specially designed for studying fundamental flame chemistry and dynamics. This study uses a coflow burner, shown in Figure 2.1b for a 2D cylindri-
cal laminar flame while the literature of counterflow burners provide the detailed chemical kinetics and extinction limits, as shown in Figure 2.1a. The coflow burner generally consists of two concentric circular tubes. The inner tube is usually where the fuel inlet flows, while the outer tube is for the oxidizer stream [19]. A counterflow burner consists of two opposing streams (fuel and oxidizer) forming a stagnation plane ($v_x = 0$) which is a quasi one-dimensional flame structure [20, 21].

2.2 Water dilution in diffusion flames

The work of Suh and Atreya mentions that water addition in a methane diffusion flame increases CO$_2$ while decreasing CO [22]. Up to 40% of water was added into the oxidizer stream of a counterflow burner maintaining the same concentration of oxygen throughout all the experiments. The turning point is that after 30% (mole percent) of water vapor added to the system the concentration of OH stays the same.
The relationship between water addition to the fuel/oxidizer and the peak concentration of OH radical has been studied by Zhao et al. [9]. A counterflow burner was used to study the addition of steam on the air side of a methane flame in numerical simulations. It was observed that when fuel and oxidizer have the same initial temperature, the concentration of OH and flame temperature decreases as steam is added.

Park et al. carry out numerical studies on the effects of water addition on the flame structure and NO$_x$ emission [23]. The numerical study consisted of the addition of H$_2$O to either fuel- or oxidizer-side on a counterflow methane diffusion flame. They showed an increase of the maximum OH mole fraction when water was added due to the reaction H$_2$O + O = 2 OH.

The work of Seiser and Seshadri consists of premixed and diffusion flames of hydrogen and methane diluted with water [24]. Both were done in a counterflow configuration on which water vapor was added on the reactants side of the premixed flames, while in the diffusion flame water vapor was added to the oxidizer stream. They conclude that in both cases, water makes the flame harder to ignite and easier to extinguish. The difficulty to sustain the methane flame is due to the production of CO in HCO + M → H + CO + M.

In the research of Wang et al., up to 40% mole fraction of water was added into the oxidizer stream of a counterflow methane diffusion flame [25]. The level of OH increases, making H do decrease and therefore CO also decreases. Water decreases the concentrations of H in the reactions O + H$_2$ = OH + H, OH + H + M = H$_2$O + M, and mainly OH + H$_2$ = H + H$_2$O. On the contrary, the reactions of OH + OH = O + H$_2$O and OH + H$_2$ = H + H$_2$O increase the concentration of OH. Also H$_2$O will increase the production of CH$_2$O by the reaction CH$_2$O + OH = HCO + H$_2$O. As for CO, the concentration will decrease in the governing reactions CO + OH = CO$_2$ + H, HCO = H + CO and CH$_2$ + CO$_2$ = CH$_2$O + CO.

The simulation of a diffusion flame from Liu et al. presented a way to isolate the chemical reactions of water addition by adding a water species that does not take part in the reactions
of combustion [26]. The effects of water vapor (up to 10 mol%) in the air stream of a laminar coflow ethylene/air diffusion flame were investigated. The study shows that the addition of water vapor to the oxidizer stream reduces flame temperature and soot volume fractions. The main reactions for the chemical effect of water are \( \text{OH} + \text{H}_2 = \text{H} + \text{H}_2\text{O} \) and \( \text{OH} + \text{OH} = \text{O} + \text{H}_2\text{O} \).

Lee et al. studies the extinction limits of a methane flame when water is added [27]. A counterflow burner was used where water vapor was added in the fuel stream. Molar ratio between \( \text{H}_2\text{O} \) and \( \text{CH}_4 \) is up to 1.4 (extinction limits). They observed a decrease in flame temperature under constant strain rates in experiments and numerical simulations. The chemical effect of \( \text{H}_2\text{O} \) on the methane flame is identified as insignificant in their work.

A coflow burner was used by Dai et al. in a numerical study to investigate the combustion characteristics of a methane jet flame [28]. Water and nitrogen was added on the oxidizer stream (up to 97 vol%) to compare the effects of the two diluents. Their findings show that the flame size and temperature decreases as water is added. Water has more effect on the production of the species \( \text{H}, \text{O}, \text{CO}, \text{OH} \) than does \( \text{N}_2 \) as a diluent. Also, by diluting water on the oxidizer, there is a lift-off of the flame.

The findings of Padilla et al. using a counterflow methane diffusion flame show that water affects the concentrations of \( \text{O}, \text{H}, \text{and OH} \) [21]. In the study, water was added up to 0.67 mass fraction and injected on the fuel side for the experimental and computational configuration. The measured \( \text{OH} \) concentration decreases at high water content in contrast with the increment of \( \text{O} \) concentration. A 3\(^\text{rd}\) body efficiency analysis of water is suggested to understand the influence of water chemical effects near the flame extinction.

Vicariotto et al. worked on the water addition in a laminar methane diffusion flame from 0% to extinction limits (70%) at atmospheric pressure [1, 16]. The study used a coflow burner for experiments and numerical simulations, where a disagreement of the flame position was
observed. The disagreement was generated from the simulations, for not predicting well the water mixing behavior, or the third body efficiency chemical effects were not captured accurately in the simulation.

### 2.3 Flame with high pressure

Pressure has a significant effect on the physical appearance of the flame. According to the law of ideal gas when pressure increases, the volume is reduced. Therefore, as the pressure raises, there are more reactants for a given volume [29]. There will therefore be more collisions and so the reaction rate is increased [8]. The higher the pressure of reactants, the faster the rate of a reaction will be. The studies of water addition at high pressure are limited, even though most practical combustion devices work in high pressures environments. As described by Matynia et al., the effect of increasing pressure during combustion is that the flame size is reduced, the flame maintains a close distance to the burner, and the flame temperature is increased [30]. An important behavior of the flame under high pressure is that most of the papers addressed the recirculation plume downstream of the flame. This is because of the instability generated by the higher buoyancy forces with increasing pressure [31]. This research is focused on non-premixed flames with elevated pressure, therefore, the following review will focus on diffusion flame studies.

A diffusion pool fire was studied by Most et al. from 0.03 to 0.3 MPa [32]. It was observed that the fire height and width were reduced, and the flames became more turbulent. The location of the flame peak temperature moved close to the burner. The pressure also influences soot formation which impacts the radiation characteristics of the flames.

The worked of Miller and Maahs [33] consisted of a high pressure flame system to study air pollution from a methane-air diffusion flames up to 50 atm with gas analyzer [33].
McCrain and Roberts study the pressure effects on the soot volume of a laminar diffusion flame [34]. At 2.5 MPa, it was observed that the flame became thinner and more concave, and the radius of the soot layer is reduced. The location of the strongest soot appearance is also shifted from the edges to the tip of the flame.

The numerical and experimental work of Liu et al. states that a coflow laminar diffusion flame becomes narrower and the flame height increases as the pressure rises from 5 to 40 atm [35]. The mass fraction of radicals H, O, and OH were observed to decrease.

Gohari Darabkhani et al. examined a diffusion flame with a pressure up to 1.6 MPa [31]. They employed propane, methane, and ethylene as the fuels and found that the flame shape changes significantly with the increase of pressure. Also, the axial flame height increases until it reaches a point where it starts to decrease with further increases in pressure. They concluded that further investigations are required due to the formation of the flame flickering frequencies as the pressure rises.

An experimental diffusion flame was analyzed at 0.5 to 4 MPa for soot formation [36]. A coflow burner with methane as fuel is tested inside a pressure vessel at 10 MPa. This is the first documented measurements under such conditions. Thomson et al. concluded that the decrease in flame temperature with the increase of pressure is due to the conversion of carbon to soot leading to heat loss from the flame to the environment. Finally there is loss from the reaction zone due to the heat conduction to the core of the flame.

Joo and Gulder conducted an extension of their prior work for, a methane diffusion flame at higher pressures (10 to 60 atm) [37]. The mass flow rate of methane remains constant at all pressures (55 mg/s). They concluded that the flame height remained unchanged under high pressure conditions. Also, soot formation has a higher dependence as pressure rises.

Escofet-Martin conducted experiments with laser diagnostics of the elevated pressure influence on a coflow methane diffusion flame at near 20 cm/s for the center fuel jet (2 mm
diameter) and a concentric air flow (40 mm diameter) [17, 18]. The pressure range of the experiment is from 1.0 atm to 11.1 atm which is the limitation of the measurable flame without pressure disturbance. The flame is observed oscillating from above 10 atm to less than 18 atm due to the design of the flow environment. The observed flame behavior with the increased pressure exhibits an unchanged flame height overall (in agreement with [37] and a decrease in OH concentration as the pressure rises [37].

2.4 Summary

Even though the dilution of water on methane flames has been studied previously, most of the dilution levels did not go beyond 40% of water content [1]. Understanding the behavior of the flame when water is added near the extinction limits (70%) can help on applications, such as combustion of methane hydrate, NOx emission reduction or fire suppression [9, 10, 12, 14, 38, 39]. The predominant reactions involved in methane combustion when water is added are listed as follows [20]:

\[
\begin{align*}
OH + H_2 &= H + H_2O \\
H + O_2 &= O + OH \\
2OH &= O + H_2O \\
O + H_2 &= OH + H
\end{align*}
\]

(2.1)  \hspace{1cm} (2.2)  \hspace{1cm} (2.3)  \hspace{1cm} (2.4)

There is an agreement that the chemical reaction \( H_2O + O = 2OH \) plays an important role for OH concentration and thus, in CO concentration. The chemical reactions most important
for the production of CO and CO$_2$ were summarized by Chien et al. [40]:

\begin{align}
H + O_2 &= OH + O \\
CO + OH &= CO_2 + H \\
CH_4 + OH &= CH_3 + H_2O \\
CH_3 + O_2 &= H_2CO + OH
\end{align}

These reactions describe the role of CO for a non-premixed flame without water addition, and its relationship with OH can further influence the emissions of combustion.

To summarize the reviewed literature on high pressure combustion, both the experimental and numerical studies of diffusion flames agree with the physical characteristics of the flame shape and size. But there is a lack of information about the influence of water content, above 40%, in the flame at high pressure and the chemical effect in the combustion of the flame. This will give us a better understanding of the effects of water for practical combustion applications. This study will focus on the analysis of these species addressed and reoccurring in the literature for water addition in high pressure conditions.
Chapter 3

Methodology

This chapter describes the numerical simulations of a laminar diffusion flame. It provides an overview of the mathematical equations, geometry, boundary conditions, initial conditions, parameters, and procedures used in the simulation.

3.1 PeleLM

Diffusion flames occur at a stoichiometric reaction interface formed between separate streams of fuel and oxidizer. In the case of premixed flames, the fuel and oxidizer, are mixed before combustion. In non-premixed combustion, important parameters are the composition of fuel and oxidizer and their input flow rates. In these simulations the oxidizer is always normal air (i.e., a mixture of nitrogen and oxygen) while the fuel is methane that is then diluted with different levels of water vapor. PeleLM is a code developed by the Lawrence Berkeley National Laboratory (LBNL) which adapts a mesh for low Mach number reacting flows [41]. The advantage of this code is that it allows the users to adjust the refinement level of the mesh and the desired location on which the calculations are made. The code is also designed
to be computationally efficient, and the results have shown a good quantification of the real value on the desired zone of the flame. In its standard configuration, PeleLM is equipped to provide information of 53 species and is also able to plot the flame with the visualization tool called AMRVIS, as shown in Figure 3.1. It utilizes the GRI 3.0 mechanism chemistry. While this mechanism is not the most recent or complete chemistry for methane, prior research has shown it to be a sufficient mechanism for non-premixed laminar flame combustion, and particularly the prior results [21] showed that the difference of major species, O, H and, OH radicals were minimal in comparison with another mechanism [42].

3.1.1 Governing equations

PeleLM solves the Navier-Stokes equations in the low Mach number regime. Here the acoustic wave propagation can be removed, allowing for much larger time steps based on an advective CFL condition [43]. This CFL factor is the Courant-Friedrichs-Lewy convergence condition necessary while solving partial differential equations. The conservation equations in the low Mach number regime is a system of advection, diffusion, and reaction processes with the following assumptions:
• Bulk viscosity is negligible.

• There are no gradients in thermodynamic pressure.

• Mixture average diffusivity is assumed.

• Dufour and Soret effects are negligible.

Therefore the governing equations for PeleLM are as follows:

\[
\begin{align*}
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu + \tau) &= -\nabla \pi + \rho F \quad (3.1) \\
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho Y_i u + F_i) &= \rho \dot{\omega}_i \quad (3.2) \\
\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho hu + Q) &= 0 \quad (3.3)
\end{align*}
\]

and:

\[
\begin{align*}
F_i &= -\rho D_{i,m} \nabla Y_i \quad (3.4) \\
\tau_{i,j} &= \frac{2}{3} \mu \delta_{i,j} \frac{\partial u_k}{\partial x_k} - \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (3.5) \\
Q &= \sum_i h_i F_i - \lambda \nabla T \quad (3.6)
\end{align*}
\]

where:

• \(\rho\), density

• \(u\), velocity

• \(\tau\), stress tensor

• \(\pi\), perturbational pressure field

• \(F\), external forcing term
• $Y_i$, is the mass fraction of species $i$

• $h$, enthalpy of the gas mixture

• $Q$, heat flux

• $\mu$, shear viscosity

• $\delta_{i,j}$, Dirac delta function

• $\lambda$, conductivity

• $T$, temperature

The $D_{i,m}$ symbolize the mixture-averaged diffusion coefficients given by:

$$D_{i,m} = \frac{\sum_{j \neq i} Y_j}{\sum_{j \neq i} X_j / D_{ij}}$$  \hspace{1cm} \text{(3.7)}$$

where:

• $X_i$, mole fraction of species

• $D_{i,m}$, binary diffusion coefficients of species pairs $i$, $j$

Conductivity $\lambda$ is given by the following formula:

$$\lambda = \frac{1}{2} \left( \frac{1}{\sum_i X_i / \lambda_i} + \sum_i X_i \lambda_i \right)$$  \hspace{1cm} \text{(3.8)}$$

The chemistry involves the interaction of $N_s$ species through a set of $M_r$ elementary reaction steps are expressed as:

$$\sum_{i=1}^{N_s} \nu'_{i,r} [X_i] \Rightarrow \sum_{i=1}^{N_s} \nu''_{i,r} [X_i] \quad \text{for } r \ni [1, M_r]$$  \hspace{1cm} \text{(3.9)}$$

with:
• $X_i$, molar concentration of species $i$

• $\nu_{i,r}', \nu_{i,r}''$, stoichiometric coefficients on the reactants and products sides of reaction $r$, associated with species $i$

Molar production rate $\dot{\omega}_i$ is given by:

$$\dot{\omega}_i = \sum_{r=1}^{M_r} \nu_{i,r} R_r$$  \hspace{1cm} (3.10)

where $\nu_{i,r} = \nu_{i,r}'' - \nu_{i,r}'$. The rate of reaction is given in terms of the forward and backward rate coefficients $k_{f,r}$ and $k_{b,r}$:

$$R_r = k_{f,r} \prod_{i=1}^{N_s} [X_i]^\nu_{i,r}' - k_{b,r} \prod_{i=1}^{N_s} [X_i]^\nu_{i,r}''$$  \hspace{1cm} (3.11)

These rate coefficients $k_{f,r}$ and $k_{b,r}$ are calculated by the Chemkin® modified Arrhenius reaction:

$$k_f = AT^\beta e^{-\frac{E_a}{RT}}$$  \hspace{1cm} (3.12)

with the parameters:

• $A$, pre-exponential factor

• $\beta$, temperature exponent

• $E_a$, activation energy

• $R$, universal gas constant

The balance of forward and backward rates are governed in the low Mach regime by the equilibrium constant $K_{c,r}$. The back reaction rate is calculated from the equilibrium con-
stant and the forward rate, and is a function only of temperature and the thermodynamic properties of the reactants and products of reaction $r$:

$$k_{b,r} = \frac{k_{f,r}}{K_{c,r}}$$ \hspace{1cm} (3.13)

with:

$$K_{c,r} = e^{\left(\frac{\Delta S^0_r}{R} - \frac{\Delta H^0_r}{RT}\right) \left(\frac{P_0}{RT}\right) \sum_{i=1}^{N_s} \nu_{i,r}}$$ \hspace{1cm} (3.14)

where:

- $\Delta S^0_r$, change in entropy of the reaction $r$
- $\Delta H^0_r$, change in enthalpy of the reaction $r$
- $P_0$, ambient pressure

The equations of conservation of energy and mass in PeleLM are solved by a coupling between advection, diffusion, and reactions. It uses the multi-implicit spectral deferred correction method (MISDC), which is one of PeleLM's unique features. This method allows for the code to take large time steps with good accuracy, even with coarse grids, avoiding numerical extinction of the flame.

### 3.1.2 Simulation domain

The flame simulation characteristics will be described briefly in this section as this research is an extension of previous work [1]. The simulation consists of a $64 \times 256$ coarse grid in a mesh of $10 \times 40$ mm in cylindrical coordinates. It is using a two-level refinement where the area of interest is the reaction zone of the flame. As seen in Figure 3.2, the boundary
conditions consist of a slip wall (right side), flame axis symmetry (left side), inlet boundary (bottom side), and outflow (top side).

The simulations reached level two of refinement after achieving steady state on prior levels. As seen in Figure 3.3, a diffusion flame is presented at three different refinement levels, with (a) a zero level refinement, where the white lines (in bold) separate the flame in different zones. These zones are the cells in which the calculations are being made. In (c) the second level refinement is represented by the red square boxes, while the green boxes are the first level refinement.

### 3.1.3 Flame ignition

The ignition of the flame begins with a blob which the simulation uses to start the flame. A blob is a high temperature (above 1000 K) object which the code uses as a spark to ignite the flame. In this work, most common blob parameters used were a temperature of 1900 K and radius of $1 \times 10^{-4}$ cm for flames with no or small water addition. As for the flames
Figure 3.3: Various refinement level on a diffusion flame at 65% water content and 5.7 atm. (a) Level 0 of refinement. (b) Level 1 of refinement. (c) Level 2 of refinement.

at higher H$_2$O content, a blob of 1300 K and radius of 2x10$^{-3}$ cm was used. This is an important aspect of the simulations and took significant trial and error because there is no exact procedure to ignite the flame. A diagram of the process to ignite a flame and achieved a steady flame can be found in Appendix A.

### 3.1.4 Burner and flow characteristics

The burner radius in the simulations consisted of a flat surface where the first 1 mm is where the fuel (methane) flows and the air is coflowing in the rest of the burner (9 mm). In between the fuel and air stream, there is a 0.2 mm layer that separates both streams to simulate the fuel tube wall. The layer will give the air inlet velocity a hyperbolic tangent profile. Details of this hyperbolic tangent profile and its impact on the simulation was studied in detail by a summer research student [44]. As for the fuel, the inlet velocity has a fully developed parabolic profile in the simulations, as seen in Figure 3.4.
Figure 3.4: Fuel and air velocity profiles with an air velocity of 0.46 m/s at 1 atm.

### 3.2 Inlet flow calculations and parameters

To evaluate the behavior of the flame, the first test consists of comparing simulation results with previous data. Therefore similar parameters are used as in [1]. Table 3.1 outlines the velocity of the fuel and oxygen at the different pressures and water content. As previous experimental results the mass flow rate of methane was kept constant at 35 ml/min in all conditions, so that the carbon input in the flame is constant for all dilution levels. Therefore the total mass flow rate of the fuel stream increases as water content rises. Pressure is constant on the whole domain, while the inlet temperature is 510 K, which matches as the experimental preheated conditions and ensures that water vapor remains in the gas phase throughout the system and the simulation [1]. Relevant water addition conditions that show the more significant results are 0, 30%, and 65% water content, and so these are the percentages tested. The selected pressure conditions from the existing experimental work for the simulations are 1, 1.4, 5.7, and 11.1 atm.

The CFL factor in the code is represented by $ns.cfl$ and the values go from 0 to 1. It is the fraction of the maximum time step allowable for the calculations to take place. As
<table>
<thead>
<tr>
<th>Mole Fraction</th>
<th>Velocity (m/s)</th>
<th>Pressure (atm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Fuel</td>
<td>Oxidizer</td>
</tr>
<tr>
<td>0</td>
<td>0.399</td>
<td>0.462</td>
</tr>
<tr>
<td></td>
<td>0.289</td>
<td>0.334</td>
</tr>
<tr>
<td></td>
<td>0.071</td>
<td>0.082</td>
</tr>
<tr>
<td></td>
<td>0.036</td>
<td>0.042</td>
</tr>
<tr>
<td>0.3</td>
<td>0.569</td>
<td>0.462</td>
</tr>
<tr>
<td></td>
<td>0.412</td>
<td>0.334</td>
</tr>
<tr>
<td></td>
<td>0.101</td>
<td>0.082</td>
</tr>
<tr>
<td></td>
<td>0.052</td>
<td>0.042</td>
</tr>
<tr>
<td>0.65</td>
<td>1.137</td>
<td>0.462</td>
</tr>
<tr>
<td></td>
<td>0.823</td>
<td>0.334</td>
</tr>
<tr>
<td></td>
<td>0.202</td>
<td>0.082</td>
</tr>
<tr>
<td></td>
<td>0.104</td>
<td>0.042</td>
</tr>
</tbody>
</table>

Table 3.1: Detailed conditions of the simulations.

The pressure increases so does the temperature on each of the cells in the grid, potentially creating an excessively high-temperature value on a cell, crashing the simulation. For the simulation to function, the value was reduced from 0.2 to 0.02 where an ignited flame was achieved.

The temperature and pressure of the simulations will affect the velocities of both the fuel and oxidizer streams because the flows are assumed to have constant mass flow rate and so continuity dictates that the velocity will change with temperature and pressure. The oxidizer stream will maintain a constant flow rate (mass flow rate equivalent to a flow velocity of 0.462 m/s at 1 atm). The oxidizer and fuel stream velocities are shown in Table 3.1. The oxidizer velocity value is selected to be able to compare with the findings of previous experimental studies of the top-hat velocity profile [16]. To maintain a constant mass flow rate the velocity of the fuel stream is adjusted by the following equation:

\[
\frac{P_1 \cdot v_1}{T_1} = \frac{P_2 \cdot v_2}{T_2}
\]

(3.15)

where \( P_1, v_1 \) are the initial pressure and velocity, while temperature \( T_1 = T_2 \).
3.3 Defining steady state

steady state is defined as a state on which the behavior of the system, in this case, the flame, does not have changes in time. In this case, the same parameter was used as in previous studies, which is when the relative error of the parameter at two-time steps 100 steps apart is 0.5% or less [1]. In order to determine the steady state of the simulated flames, the concept of relative error formula was used:

\[
Relative Error = \frac{\| I - R \|}{\| I \|} \times 100\% \tag{3.16}
\]

The relative error represents the error between the real value (R) and the expected or ideal value (I). In the simulation, there is no ideal or real value to compute, but there is a continuation of new value predicted with time step progression. Therefore, the definition of steady state in this work is comparing between two-time steps using the following formula:

\[
Relative Error = \frac{\| V_i - V_{i-100} \|}{\| V_{i-100} \|} \times 100\% \tag{3.17}
\]

\( V_i \) represents the predicted value at the final time step of the variable of interest. The variable can be the species’ mass concentration or the temperature of the flame. \( V_{i-100} \) is the value 100 time steps earlier. The time step reaching a steady state is when the relative error is less than 0.5%. This method is used for all of the variables at each time step while PeleLM reports the maximum relative error for each variable. PeleLM does not have a fixed time step with respect to the physical time scale because of how the code solves the governing equations to be efficient and decrease computational time, but every 100-time step in the simulation is around, 1.5 ms and 3 ms in physical time. As mentioned previously, the relative error determines the steady state of the diffusion flame when the species mass concentration results in a relative error equal to or less than 0.5%. The time step after 0.5% is the one used to evaluate the results. If the simulation is kept running, the relative error will decrease
and the results will change. For example, for the flame maximum temperature in the case of 65% water content at 1 atm, if the simulation continues running after reaching a relative error equal to 0.5%, the relative error value keeps decreasing below 0.5%. This produced a result of up to 5 degrees Kelvin of difference between the time step after 0.5% (real-time 932 ms) is achieved and the last time step (real-time 1042 ms) after the simulation has been stopped. The flame maximum temperature will reduce 3.3 K for every 110 ms of the running simulation after reaching a relative error of 0.5% and will do so until it stabilizes. Precisely, to have a validated comparison between the water addition cases, the results obtained from the initial time step and the value obtain 100-time steps later has to be a relative error of at least 0.5% and less.

In the cases of the flames at 11.1 atm with or without water addition, the steady state could not achieve a relative error equal to or below 0.5% on all the species due to the oscillation of the flame plume, as seen in Figure 3.5. This is because the buoyancy force of the flame is increasing with the pressure rise, which leads to buoyancy-induced instabilities and flame flickering [17, 31, 34]. For these higher pressure cases at 11 atm, the convergence is targeted in observing physical properties such as temperature, density, and the concentration of the six species highlighted in this research instead of all the variables.

### 3.4 Summary

This chapter described the numerical simulations using PeleLM software and the detailed settings along with the modeling principles. The domain and the parameters were described to simulate a methane diffusion flame in cylindrical coordinates. It is important to emphasize that the ignition process of the flame did not affect the flame results, but it is a procedure that is required as a key step to initiate the simulation studies. In the next chapter, the results
Figure 3.5: The methane flame jet with coflow air instability at 65% water content at 11.1 atm.

Of these simulations, such as maximum flame temperature and concentration of species will be presented.
Chapter 4

Results

To evaluate the results given by PeleLM such as species concentration and maximum flame temperature, this chapter includes the results from the simulations of a diffusion flame for water and increasing pressure from 1 to 11.1 atm. All of the physical property results acquired are taken along the centerline toward downstream of the flame. This line represents the center of the flame as seen in Figure 4.1. This will help understand the behavior and the role of water when added to a methane diffusion flame.

4.1 Simulation validation

The simulation results for the water addition of PeleLM code were first validated with previous results from the experiment and computation [1], and the pressure results will also be validated with existing experimental data [17, 18]. The prior water addition work was conducted with experiments at atmospheric pressure along with some initial simulation efforts with PeleLM. This thesis lists three cases of water addition concentrations (0%, 30%,
and 65%) in atmospheric condition to first learn the difference between the experiments and between the methods of running the code as the baseline understanding.

The peak flame temperature is used to compare with previous studies as the representation of the reaction zone. The plot is shown in Figure 4.2. The result of 30% water addition case has a close match within 0.07% with the previous simulations, and 1.8% and 1.3% for 0% and 65% water content cases respectively. The detailed temperature in Kelvin is tabulated in Table 4.1. From an overall perspective observing from 0-65% water addition, the temperature differences between this work and the previous PeleLM simulation are approximately 40 K and 25 K respectively. This represents 1.3-1.8% of the overall flame temperature (at around 2000 K). It is noticed that both of the simulated peak temperatures from PeleLM are higher than the in-lab measurements, and this is attributed to losses of heat in the experiment not captured in the simulation [1].

Figure 4.1: Diffusion flame were the red line marks the extracted results.
Figure 4.2: Comparison of maximum flame temperature of the simulations from this study and experimental values and simulations from Vicariotto [1].

Table 4.1: Detailed temperatures in Kelvins.

<table>
<thead>
<tr>
<th>Water addition mole fraction</th>
<th>Experimental</th>
<th>Temperature (K)</th>
<th>Relative Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2093.2</td>
<td>2136</td>
<td>2.0</td>
</tr>
<tr>
<td>0.3</td>
<td>2028.8</td>
<td>2087</td>
<td>2.9</td>
</tr>
<tr>
<td>0.65</td>
<td>N/A</td>
<td>1955</td>
<td>N/A</td>
</tr>
</tbody>
</table>
4.2 Water addition and pressure effects on flame appearance and temperature

In this section, the water addition and pressure effects on the flame appearance and maximum temperature are discussed by comparing them with previous results. As mentioned in the literature, water addition will have thermal effect [16], meanwhile the pressure effect will reduce the flame size [17, 45]. From the data obtained from PeleLM, temperature contour plots for the flames are shown in Figure 4.3. The images were zoomed-in for a clear view of the differences. These contour plots present the flame under the conditions when water is added (0%, 30% and 60%) and pressure is increased (1 atm, 1.4 atm, 5.7 atm, and 11.1 atm). The 65% water addition case at 1 atmosphere, the flame is lifted from the burner tip, which is also observed in previous studies because of the increase of the total mass flow [16].

One of the main factors of water addition into the flame is the thermal effect on the maximum temperature within the reaction zone. As seen in Figure 4.4, the data trend shows that the peak temperature decreases when water is added. This correlates with the findings in the past studies [1, 16, 28]. There is a relatively more significant reduction of the peak flame temperature from 0.30 to 0.65 water addition than from 0 to 0.30 water addition. For all the pressure conditions, the peak temperatures at 0.65 of water addition are averaged around 200 K less than the flames with no water addition.

The pressure effect on the flame can be seen clearly at 11.1 atm, as shown in Figure 4.3. The work of Escofet-Martin et al. gives a baseline of high-pressure flames without water addition [17]. As for the current work, those experiments and other results in the literature show that the flame size reduces with elevated pressure and a more sharp edge is formed [35, 45]. The width of the flame reduces, losing its round shape when pressure is elevated. At the 65% water content condition, as the pressure starts to increase the flame reaction zone moves back to the burner tip. The overall pressure influences on flames at 0% and 30% water content are
Figure 4.3: Temperature of all flames under different conditions.
Figure 4.4: Maximum temperature vs. water added of all cases.

Figure 4.5: Maximum temperature vs. pressure of all cases.
relatively insignificant when compared with the flame at 65% water content. A recirculated plume downstream is observed at 11.1 atm. This is due to the instability generated by the higher buoyancy forces with increasing pressure [31, 34]. At the same water addition content, the peak temperature increases with increasing pressure as seen in Figure 4.4.

4.3 Species

This section includes the result of the effects of pressure and water addition, and the result of the species involved. These species are H$_2$O, CO, CO$_2$, H, O, and OH. The physical appearance of the concentration of these species in the flame can be seen in Figures 4.6, 4.7, 4.8, 4.9, 4.10 and 4.9.

4.3.1 CO, CO$_2$ and H$_2$O concentration

The species presented here are H$_2$O, CO, and CO$_2$. As seen in Figures 4.12 and 4.13, the maximum concentration of CO and CO$_2$ for the three water addition cases are presented against pressure. It is observed that CO and CO$_2$ concentration increases when pressure rises but the addition of water inhibits the formation of these two molecules. It is important to note that the concentration of CO at 65% water content (blue dash line) decreases from 1 atm to 5.7 atm, as seen in figure 4.12. The drop of CO concentration from 1 to 1.4 atm (blue square) is greater than 1.4 to 5.7 atm, which is presented in all three different water content conditions. As for CO$_2$ in Figure 4.13 there is a big difference in the maximum concentration of the water addition case of 30% (black dash line) and 65% case (blue dash line). Between the pressures of 1 and 1.4 atm, there is no decrease in concentration. On the contrary, there is an increase. Pressure has a positive effect on the maximum concentration of CO$_2$ and a negative effect on CO.
Figure 4.6: CO$_2$ concentration for all conditions.
Figure 4.7: CO concentration for all conditions.
Figure 4.8: H$_2$O concentration for all conditions.
Figure 4.9: OH concentration for all conditions.
Figure 4.10: H concentration for all conditions.
Figure 4.11: O concentration for all conditions.
Figure 4.12: Maximum mole fraction concentration of CO in all cases.

Figure 4.13: Maximum mole fraction concentration of CO\(_2\) in all cases.
Figure 4.14: Comparison of mole fraction of H$_2$O, CO and CO$_2$ species at 11.1 atm at 1 cm of height.

Following the species in the centerline of the flame, Figure 4.14 shows the mole fraction of H$_2$O, CO$_2$ and CO at 11.1 atm are plotted in comparison with the water addition of 65% (solid line), and 0% or 30% (dash line). The concentration of CO$_2$ stays similar at 0% and 30% water addition, suggesting that H$_2$O has no effect in CO$_2$. On plot (a) from the distance 0.3 to 0.4, the concentration levels of CO are higher than CO$_2$ at 0% in contrast to the same position in the plot (b) where the concentration of CO does not even reach the same as CO$_2$ at 30%.

Figure 4.15 shows the temperature data along the centerline away from the burner toward downstream of 1 atm and 11.1 atm for 0% water addition, and the dash line represents 65% water addition for 11.1 atm. In the distance from 0.2 to 0.4 cm an uphill can be seen and another at 0.5 to 0.8 at 0% water content. At 65% water content, this uphill is decreased and shifted upward. The character of the two-stage temperature gradients observed from 11.1 atm demonstrates the heat release from the reaction zone is compacted with density enhancement. As seen in Figure 4.16, the case of 65% water content and 11.1 atm the concentration of CO$_2$ (red dash line) follow the path of the temperature profile. The decrease of CO$_2$ at the distance 0.2 and 0.4 could be explained by the increase in CO (blue
Figure 4.15: Temperature data along the centerline away from the burner for 1 and 11.1 atm (solid lines) for 0% water content. The dash line is 65% water content for 11.1 atm.

dash line) concentration. The reaction rate will determine the speed at which a chemical reaction will take place. Temperature, concentration, the physical state of reactants, and the presence of catalyst are factors that affect the reaction rate. As the temperature rises, molecules move faster and collide more vigorously, therefore the higher the probability that molecules will be moving with the necessary activation energy for a reaction to occur upon collision [20]. The temperature will rise with pressure because collision frequency increases and when there is a higher reactant concentration, more reactions will occur. Hence in high pressure for diffusion flame, the increase of CO and CO$_2$ is expected while water addition also plays a role of enhancing oxidizers to the level of lifted flame (overventilated flow) with either a diluted species concentrations or temperature reduction.

To examine the chemical reactions of the species, the maximum mole fraction concentration of CO$_2$ in the flame was located and compared to the concentration of CO and H$_2$O in the same spot. The results are shown in Figure 4.17. The gap between water concentration (black dash line) and CO$_2$ (blue dash line) increases significantly. However, in comparison
Figure 4.16: Temperature profile and concentration of CO\textsubscript{2} and CO at 65% water content and 11.1 atm.

between the gap of CO\textsubscript{2} and CO (red dash line), it stays the same. The concentration of CO changes in a small amount between 5.7 and 11.1 atm.

Figure 4.18 shows the maximum concentration of water in all the conditions at 1 (a) and 11.1 atm (b). For all three conditions, water concentration experienced an increase between 0.4 to 0.6 (black and red line) and 0.6 to 0.8 (blue line) in Figure (b). Unlike (a), there is no clear increase of water concentration as the flame starts forming, only that the concentration decreases.

Figure 4.19 shows the temperature, H\textsubscript{2}O, CO\textsubscript{2}, CO and O\textsubscript{2} mole fraction along the radius of the flame at the height of the peak temperature. Here CO mole concentration is multiplied by 10 to have a clear vision of its behavior. Previous section 3.3 (Figure 3.5) has addressed the buoyancy-induced instabilities at 11.1 atm leading to entrained airflow near the coflow stream. The temperature profile at 11.1 atm along the radius in Figure 4.19 demonstrates a region outside the flame edge that has a lower temperature value than the initial temperature at 510 K. This can be attributed to the wall boundaries, other boundary conditions settings, high-pressure instabilities, or any other computational conditions that lead to the local
ambient airflow (at 300 K) entraining into the coflow air region and stagnating there. Further investigation is needed into this anomalous temperature while this research will continue the discussion focusing on the flame region. It is observed that the CO is reduced with water addition and this reduction is particularly clear at higher pressure conditions. At 65% water content Figure 4.20 show a comparison between the cases at 11.1, 5.7 and 1.4 atm. In Figure 4.20a the difference in temperature and species concentration is higher than in Figure 4.20b.

### 4.3.2 OH, O and H concentration

The species considered in the reactions are O, H, and OH. These species play a role in the reaction process of the combustion of methane, water, and emission of gases such as CO and CO$_2$. Overall, the OH concentration decreases as the pressure rises, as seen in Figure 4.21.
Figure 4.18: Comparison of mole fraction of H$_2$O under 0%, 30%, 65% water content at 1 and 11.1 atm.
Figure 4.19: Temperature and species mole fraction along the flame radius. CO concentration is x10 for all of the conditions.
Figure 4.20: Comparison of temperature and mole fraction of O$_2$, H$_2$O, CO$_2$ and CO under 65% water content at 1.4, 5.7 and 11.1 atm. CO concentration is x10 in the plots.
This is the same when water is added at atmospheric pressure which contradicts the studies mentioning that OH increases with more water vapor addition [22]. However, the results obtained are in agreement with the findings by Padilla et al. [21]. Without water addition (red dash line) the drop of OH concentration from 1 atm to 11.1 atm is significant. The same happens when water is added (black and blue dash line). OH predominant reactions with water are \( \text{H}_2\text{O} + \text{H} = \text{OH} + \text{H} \) and \( \text{H}_2\text{O} + \text{O} = 2 \text{OH} \) [21, 35, 46], as for with CO are \( \text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O} \), \( \text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H} \), \( \text{CH}_4 + \text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O} \), \( \text{CH}_3 + \text{O}_2 \rightarrow \text{H}_2\text{CO} + \text{OH} \) [40]. The changes in these reactions as the temperature fall with water addition could help explain the decrease in OH concentration.

As seen in Figures 4.21, 4.22 and 4.23 pressure decreases the maximum concentration of H, O and OH. The same effect is seen with the addition of water at 65% water content. In Figure 4.22 at pressures levels of 5.7 and 11.1 atms and 65% water content (blue dash line), the concentration of O barely has any changes. This also apply to Figure 4.23, where H maximum concentration is displayed, Hence this suggests that pressure does not have a role in chemical reactions involving water. The concentration of the species of O and H was analyzed in the same region where OH is at its maximum value. Figure 4.24 represents the maximum value.
Figure 4.22: Maximum mole fraction concentration of O in all cases.

Figure 4.23: Maximum mole fraction concentration of H in all cases.
of OH (red dash line) of all different conditions and the values of O (blue dash line) and H (black dash line) at the same point. This continues with the result that pressure and water decrease OH concentration. In the first section of 0% water addition, there is an increase of H (blue triangle) from 5.7 to 11.1 atm, despite H concentration decreases on the other conditions. When water is added (30% and 65%) at 5.7 and 11.1 atm, the concentration of O and H becomes nearly equal.

In order to see a clear distribution of these species at the same height along the radius, Figure 4.25 shows the temperature, OH, H, and O mole fraction along the radius of the flame at the height of the peak temperature. The result shows OH peaks near and within the peak temperature region while O and OH are consumed earlier in radius at higher pressure conditions. Figure 4.26 shows the ratio between the OH, O, and H mole fraction species of all cases and the mole fraction at equilibrium. The mole fraction at equilibrium

Figure 4.24: Maximum concentration of OH on the flame.
is computed using the Colorado State University online calculator (that is based on the original Stanjan Equilibrium Code) for the conditions of 0%, 30% and 65% water addition to a stoichiometric fuel/air mixture [47]. The ratio of, for example, $\frac{\text{H}_{\text{this work}}}{\text{H}_{\text{eq.}}}$, presents the ratio between the equilibrium prediction and the kinetics result for these atoms at all the pressure conditions. The results show that H and O have a consistency of more than two times over equilibrium for all water content at lower pressure, while OH stays near the equilibrium value throughout all the conditions in this research.

4.4 Summary

The results of the simulations were presented in the form of the flame peak temperature and the maximum concentrations of the species $\text{H}_2\text{O}$, $\text{CO}_2$, CO, H, O, and OH. The results were compared to past studies to validate the simulation. The flame peak temperature increased when pressure rises, however water addition decreases its value. This same description applies for CO and $\text{CO}_2$ concentration, despite seeing a drop in concentration for CO when pressure begins to rise. Pressure and water addition decrease the concentration of H, O, and OH. Having a higher concentration of one reactant, in this case, water, the reaction rate will increase favoring those reactions in which $\text{H}_2\text{O}$ is involved. The relationship of reaction rate, pressure, and temperature may explain the concentration development of the different species. There is an increase in the activity of the molecules as pressure rises, proof of this are the species as H, O and OH which, played an important role in combustion processes, decreases in concentration.
Figure 4.25: Temperature and species mole fraction along the flame radius.
Figure 4.26: The mole fraction ratio of the PeleLM calculation and the equilibrium of OH, O and H species from low to high pressures at each water content.
Chapter 5

Conclusion

Numerical simulations of laminar methane diffusion flames were carried out at high-pressure conditions (1.4, 5.7, and 11.1 atm) and three water content levels (0%, 30% and 65%). Water addition has been researched previously, but little has been done with high water content or in elevated pressure. Most of the existing experimental and computational works are far below the extinction limits of the flame with water concentration and are done at atmospheric pressure. This study is particularly focusing on the role of water in the combustion of a methane diffusion flame spanning from low to high water content and also at high-pressure conditions.

The simulations were carried out with an open-source code PeleLM for solving the Navier-Stokes equations of low Mach number reacting flows. This code allows the adjustment of the refinement level of the mesh and the desired location on which the calculations are made with supercomputation parallel capability. A methane diffusion flame was generated in cylindrical coordinates with a course grid of 64 x 256 coarse grid in a mesh of 10 x 40 mm.

Results of flame peak temperature and various species concentrations were determined with different water content and pressure conditions. The simulation code and strategy of this
work were first validated with the existing data with the peak flame temperature. In general, it is known that water addition decreases the flame peak temperature, and elevated pressure influences flame shape, increases the flame peak temperature, reduces the distance from the base of the flame to the burner tip, and creates buoyancy induced instabilities in the flame. However, there have not been studies when these two factors are introduced at the same time. At 11.1 atm, the flame forms a more conical shape and the width reduces. 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, water addition decreases the flame peak temperature and lifts the flame away from the burner tip.

The maximum mole concentration of CO\textsubscript{2} and CO were also investigated for all conditions. CO\textsubscript{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. H\textsubscript{2}O 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. As for the species O, H, and OH, pressure and water addition decrease the maximum mole concentration in all conditions. From 5.7 to 11.1 atm the decrease in maximum concentration is not as high as from 1 to 5.7 atm. The maximum mole concentration of H and O are similar at high-pressure conditions in contrast to atmospheric pressure. The decrease of OH for water addition and particularly at higher pressure leads to less CO in the reaction zone and can impact the resultant concentration of NO\textsubscript{x} or soot. These results outline the behavior of the flames at high pressure when water is added under three conditions.
5.1 Future work

Water is one of the diluents most commonly used which has a significant effect on the flame properties. CO$_2$ has also been used as a diluent in flue gas recirculation applications, and therefore it is a possible path in exploring the influences on methane diffusion flame. The other diluents such as argon can be explored to see the effects on flame behavior. Chemical reaction pathway analysis should be made to identify the reactions that are responsible for the difference in mole concentration of the species mentioned in this research. Also, seeing the behavior of other species such NO$_x$ or CH can add more insight into the effects of water addition. Further analysis together with the existing high-pressure experiment results (with no water addition) and on the superequilibrium prediction for the species (H and O) at low pressure are required as a reliable validation of this study.
Bibliography


Appendix A

Logic flow diagram of the simulation process from ignition to steady-state