Review Paper

Simulation Combustion of Natural Gas

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Abstract: During combustion, natural gas can improve the characteristics of combustion and reduce carbon emission, which has important engineering application value. The simulation approach which was used for the problem in 2D axi-symmetry steady state turbulent model with species transport equation. The use of a 2D axi-symmetric model reduces the workload on the computational source and will reduce the time required for simulation. Under the condition the temperature distributions, composition, and emission of combustion flue gas under various working conditions are analyzed and compared. Further investigation is also conducted for the variation laws of NOx and soot generation. This study shall help to reduce the time spent in an investigation as the use of computation and save time and money in expensive experiments. Also, it's useful to study NOx emissions in combustion systems.

Keywords: simulation combustion; combustion characteristics; soot generation; flue gas analysis

1. Introduction

We are all aware of burning, Combustion is actually a scientific term for burning. Combustion is a chemical reaction between Fuel (Hydrocarbon) and Oxygen. When fuel and oxygen react it releases the heat and light energy. Heat and light energy then result in the flame. Combustion is a very important part of our daily lives and the main source of heat used in the industry. The next paragraphs can illustrate some of these reasons.

Firstly, as a main source of energy, to maximize the efficiency of the combustion systems and obtain the maximum profit from the resources. Secondly, it is not just the concern about efficiency that boost the studies about combustion. We make these processes must be environment-friendly and the most limiting aspect for the optimization of the combustion systems is the pollution associated with it. These gasses (NOx, SOx, CO, CO2) are directly related to global warming. So we have a strong reason to spend resources in technology to improve the combustion systems.

On the other hand, computational resources are increasing at an astonishing rate, which allows us to perform simulations in such detail and velocity that was very difficult a few years ago. Also, this allows to reduce the time spent in an investigation for a first approach and save time and money in expensive experiments.

This final project is intended to use the advantages resulting from the availability of CFD software with ANSYS-Fluent and apply it to the study of NOx emissions in combustion systems.

2. Objective

The objective of this work is the study of NOx formation in systems by using a commercial CFD software called ANSYS:Fluent. In order to carry out this study, the work has been divided in some specific, measurable, achievable, realistic and time-based objectives. Those objectives are:

1. To study the combustion phenomenology.
2. To study eddy dissipation models.
3. To study the NOx and shoot formation inside the burner.
4. To pre-process the geometry for the simulation.
5. To select the correct element size and type for simulation.
6. To plot the mass fraction of C02, H2O, CH4, N2, O2, NOx and shoot formation.

3. Spaceclaim Model

The Materials and Methods should be described with sufficient details to allow others to replicate and build on the published results. Please note that the

Figure 1 Combustion Model

- This is 3D model, we can't run simulation for entire 3D model, it will cost lot interims of time.
- So instead of 3D, we will perform simulation on 2D geometry, which is Axis-symmetric.
- For 2D geometry we have to cut 3D model in two parts, and extract 2D geometry of the quadrant portion.

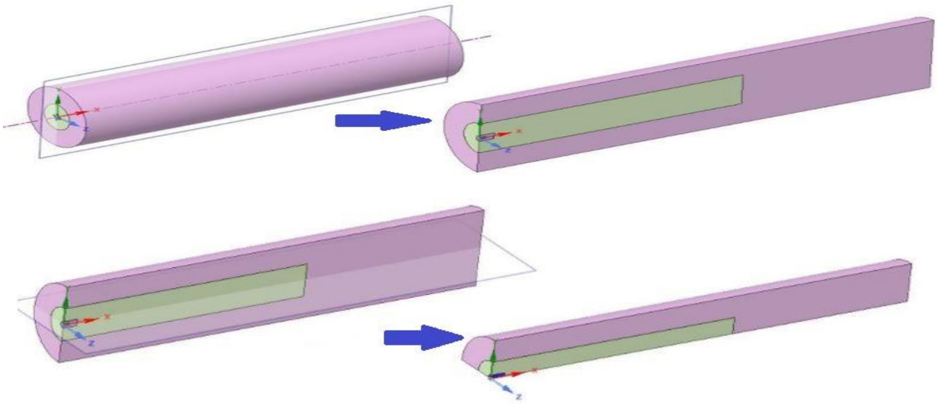


Figure 2 All Model faces from X-Y plan

- Then we copy all faces from X-Y plane and paste it in New Design.
- Then we paste it only in X-Y plane.
- After pasting, we merge all faces by using 'combine' command and can make it a single surface.
- So the 2D geometry can be ready for further process.

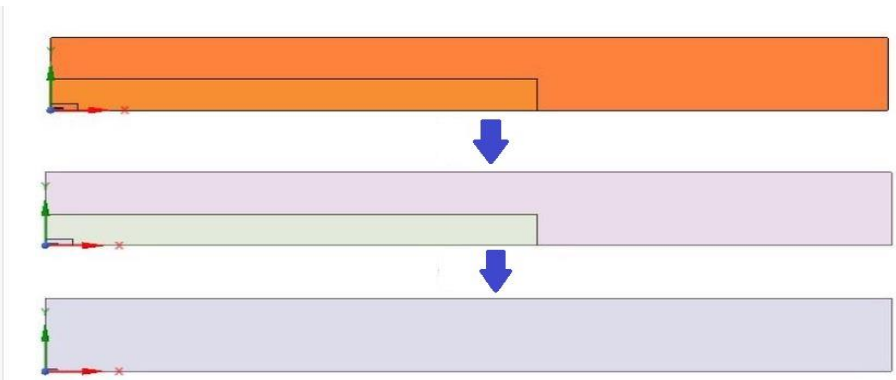


Figure 3 2D Geometry

4. Computational Fluid Dynamics: ANSYS-Fluent

In ANSYS Software CFD simulation provides a virtual laboratory to perform experiments in the early stages of design without building the physical apparatus. Using these virtual laboratories we can decrease the unit design costs as the number of unsatisfactory experimental devices that ends to scrap decrease drastically. And Because of this the cost of the experimental device and its operation until obtaining satisfactory results can become very huge. CFD simulation real solution accuracy depends on the appropriate selection of the models.

4.1 Performing a Simulation in ANSYS-Fluent:

ANSYS is a software suite that provides access to lots of fields of engineering simulation that a design process requires. Module FLUENT is appropriate for this work. FLUENT's models are focused on fluid flow and chemical reactions, including a very good model to run first-approach simulations of combustion systems.

So we are ready to perform a simulation using ANSYS: Fluent. Starting, but not focusing, on the geometry and mesh creation, and continuing on how to set up the models and run the calculations. At this time we studied the combustion of methane in air, in turbulent flow, and using a simple reaction mechanism. Once it's achieved, we are ready to simulate the effect on the NOx formation.

To perform a simulation in ANSYS FLUENT, the next steps are followed:

4.1.1 Geometry Design

Figure 5 provides the configuration and dimensions of the combustion chamber used in the simulations as well as the fuel and air rates passing through the system. Due to the high level of symmetry present in the system, the calculation domain can be reduced to a 2D problem assuming no variations in the radial coordinate. If done, the computational time required for the calculations decreases drastically.

4.1.2 Mesh Generation

In the combustion chamber, the mesh must be refined all long near the center (symmetry axis) and close the fuel inlet, because there is where the combustion reaction occurs. the combustion chamber has been discretized using ANSYS's own meshing program, introducing a sphere of influence and an inflation ratio to refine the mesh in the important zones of the system. In the figure below, is presented a view of the sphere of influence, and the final mesh used for the calculations with the sphere and inflation applied.

1. Element Size: 1 mm
2. Method: All triangle Method
3. Numbers of Nodes: 73670
4. Numbers of Element: 145540

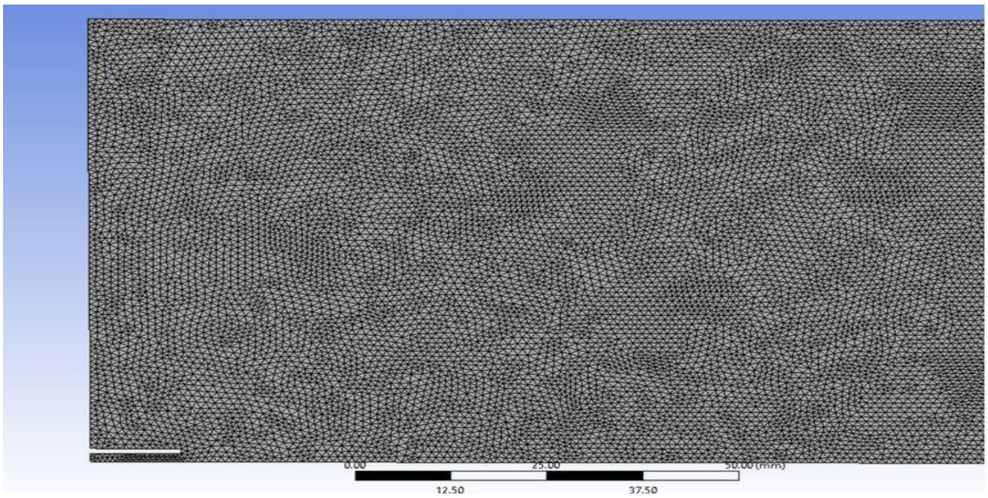


Figure 4 Mesh Setting

4.1.3 Simulation Setup

ANSYS has some valid applications available that could solve the problem posed in this work. The software ANSYS FLUENT has been selected because it incorporates a good package for simulating the combustion phenomena. Inside FLUENT the setup consists in the following parts, necessary to perform the calculations.

1. Solver: Steady
2. Type: Pressure Based
3. Turbulence Models: Standard k-epsilon with Standard wall function
4. Energy Model: On
4. Species Model: Images

5. Combustion Analysis & Reaction

The general combustion requires fuel, air, and activation energy and it produces vapor and flue gas, which is the emission that we want to reduce. In this paper, a simple natural gas fuel composition was used that contained methane as the main component besides carbon dioxide, nitrogen, ethane, propane, butane, and pentane.

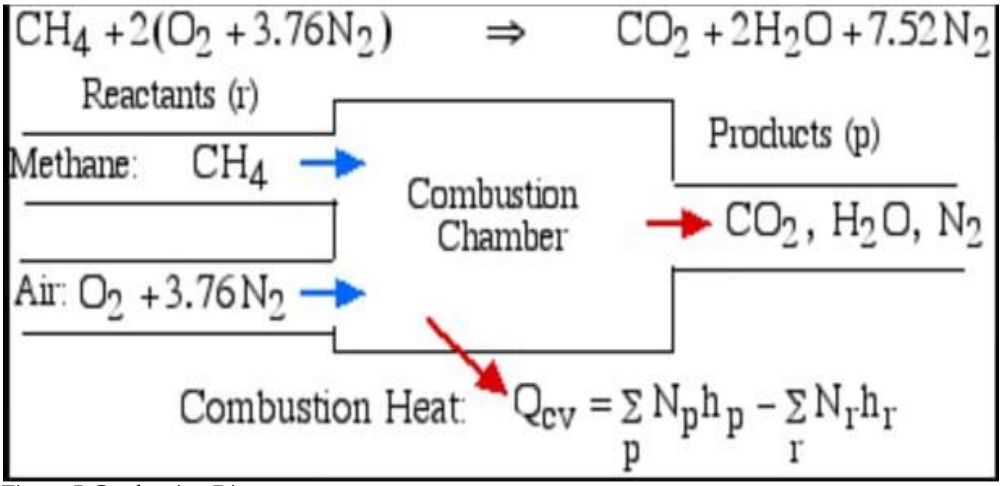


Figure 5 Combustion Diagram

The general reaction of combustion is given as follow:

CH4 + ar(O2 + 3.76 N2) = aCO2 + bH2O + cN2

Balancing- a=1, 2b=4, b=2, 2ar=2a+b, ar=2, c=7.52ar and c=15.04

6. Boundaries:

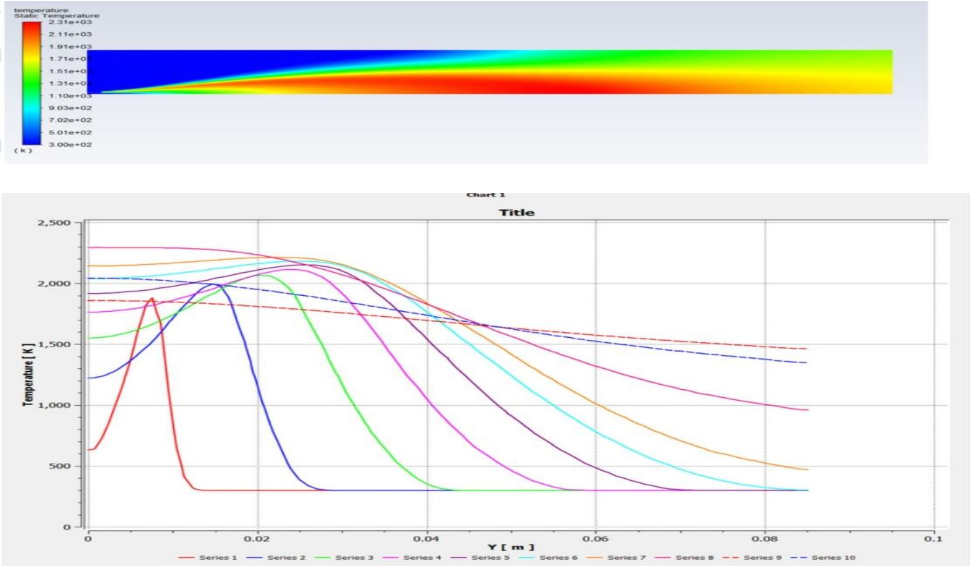
The Boundaries of the geometry are generated using the named selection feature of ANSYS,
Axis
Fuel inlet
Air inlet
Walls
Outlet

7. Result

The most important parameters involved in the NOx formation as described in the previous section are the temperature, and the O, H and OH radicals' concentration. If we do a visual analysis of the system, in the next pages the profiles of these parameters for each of the simulations of the sensitivity analysis are presented.

7.1 Part 1

Temperature Contour



CH4 Mass Fraction

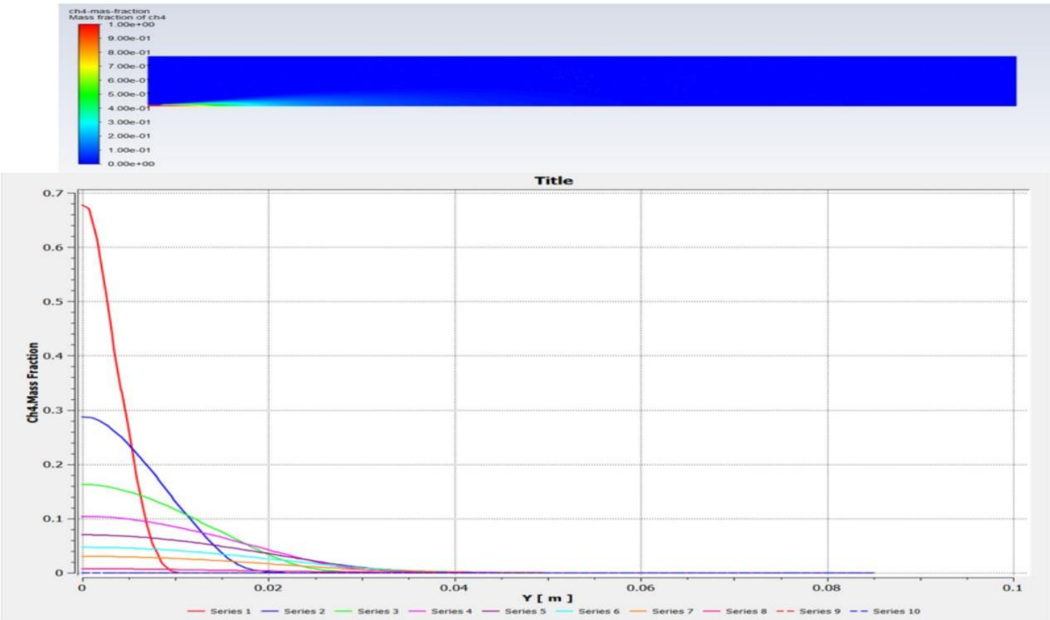


Figure 6 CH4 distributions

CO2 Mass Fraction

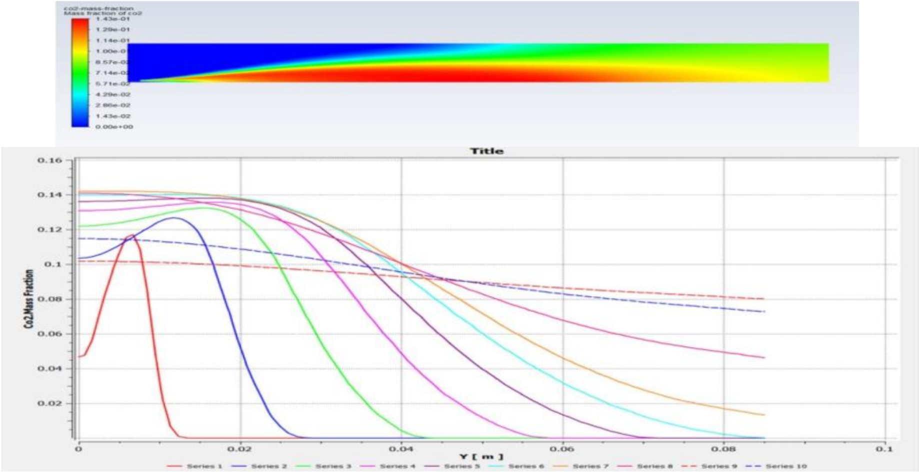


Figure 7 CO2 distributions

O2 Mass Fraction

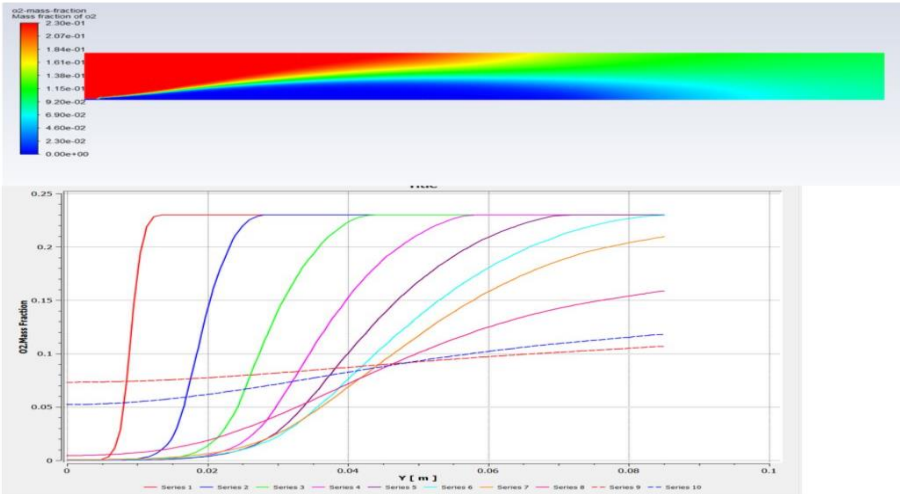


Figure 8 O2 distributions

N2O Mass Fraction

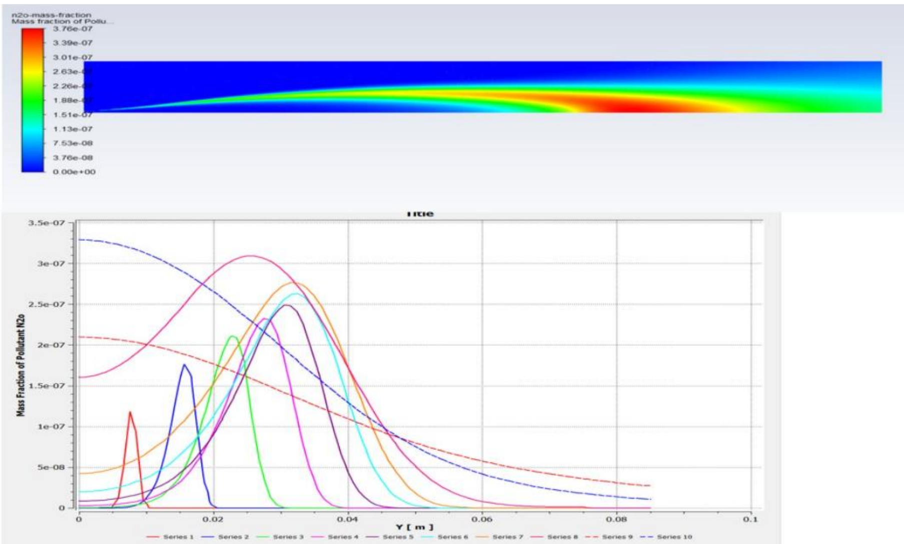


Figure 9 N2O distributions

H2O Mass Fraction

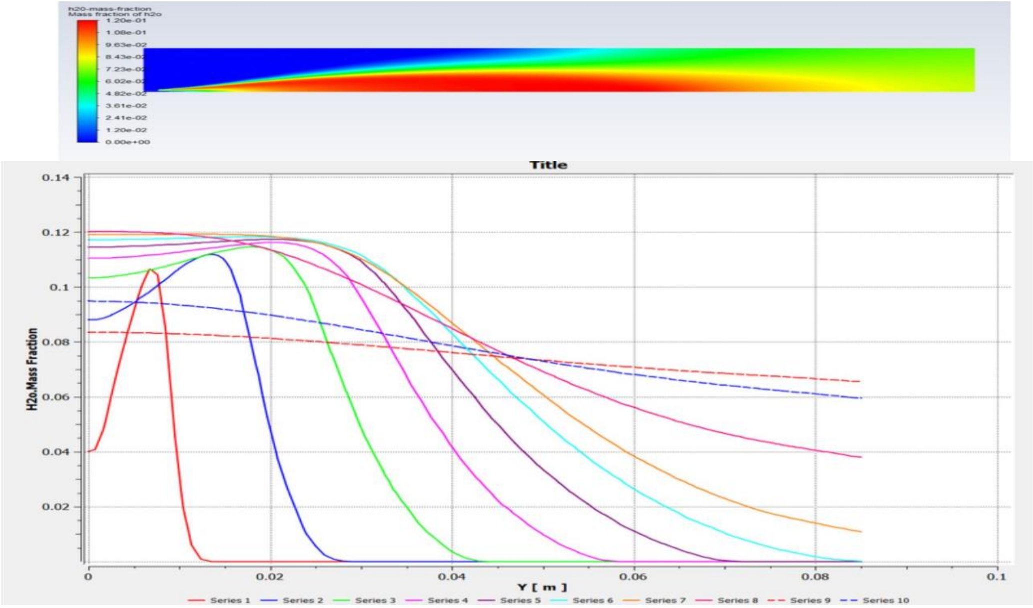
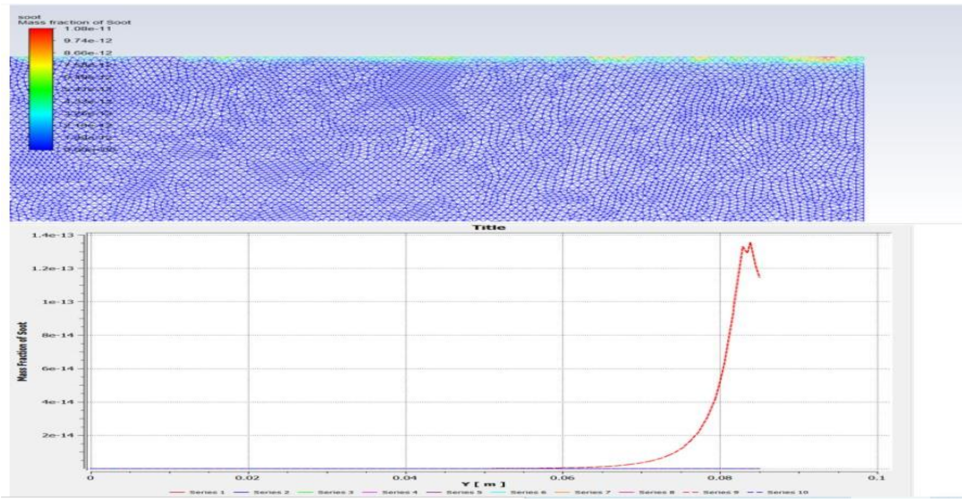


Figure 10 H2O distributions

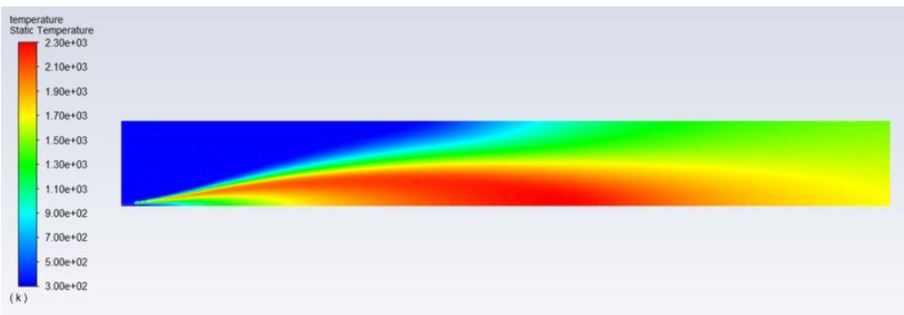
SHOOT Mass Fraction



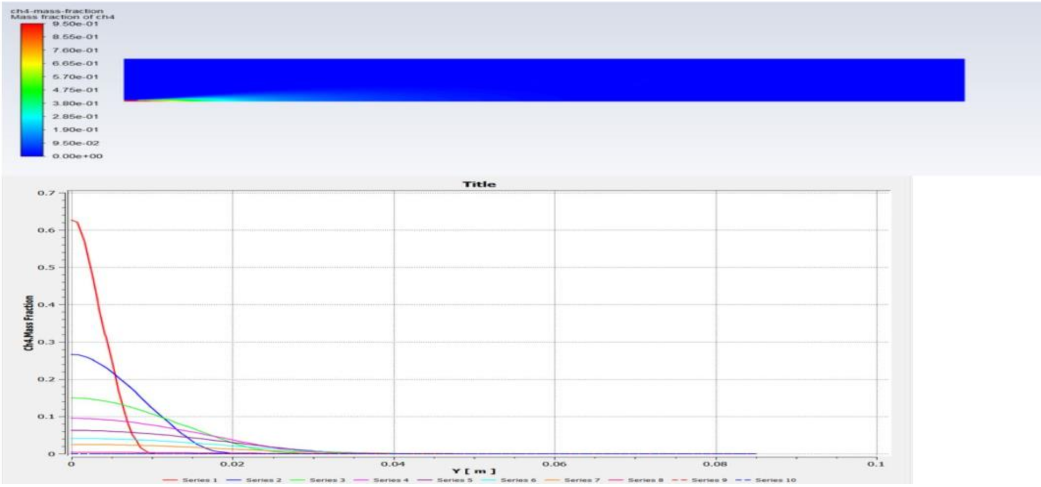
7.2 Part 2

7.2.1 CASE 1: 95% CH4 and 5% H20

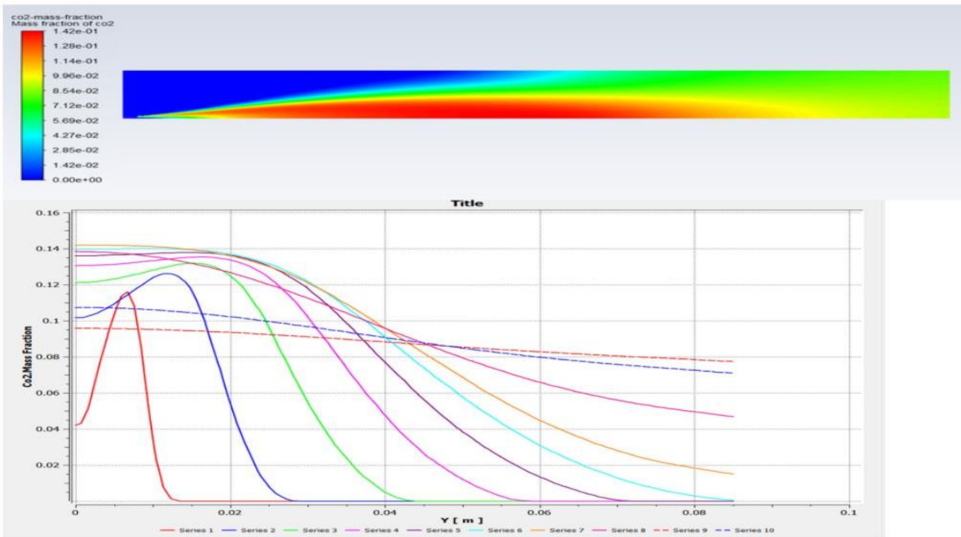
Temperature Contour:



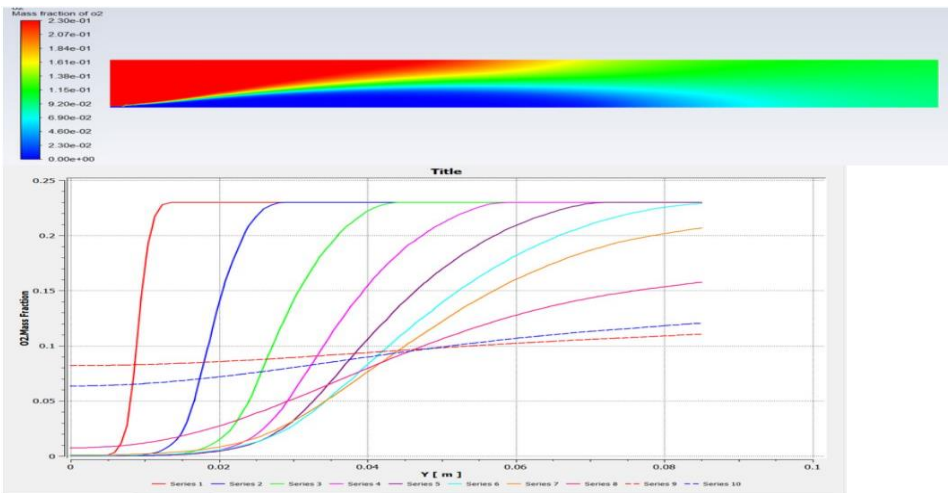
CH4 Mass Fraction



CO2 Mass Fraction



O2 Mass Fraction



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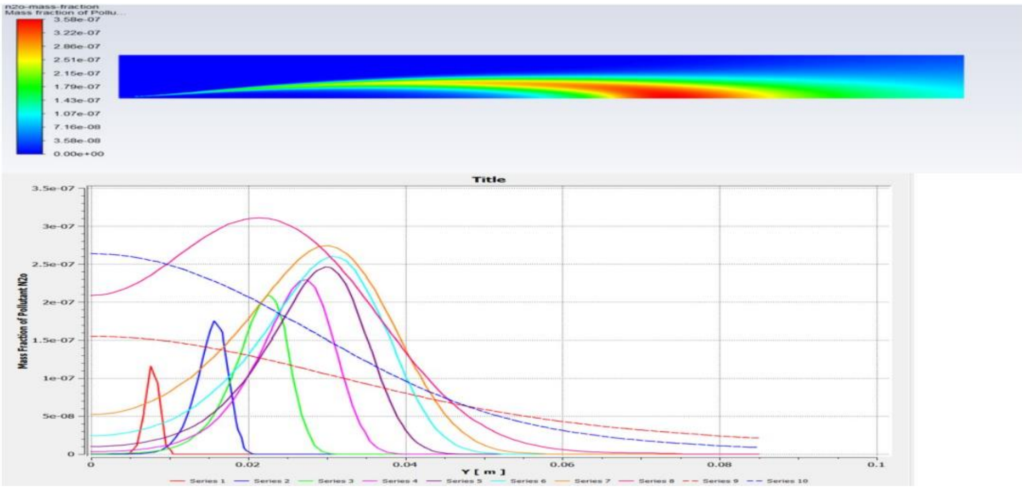
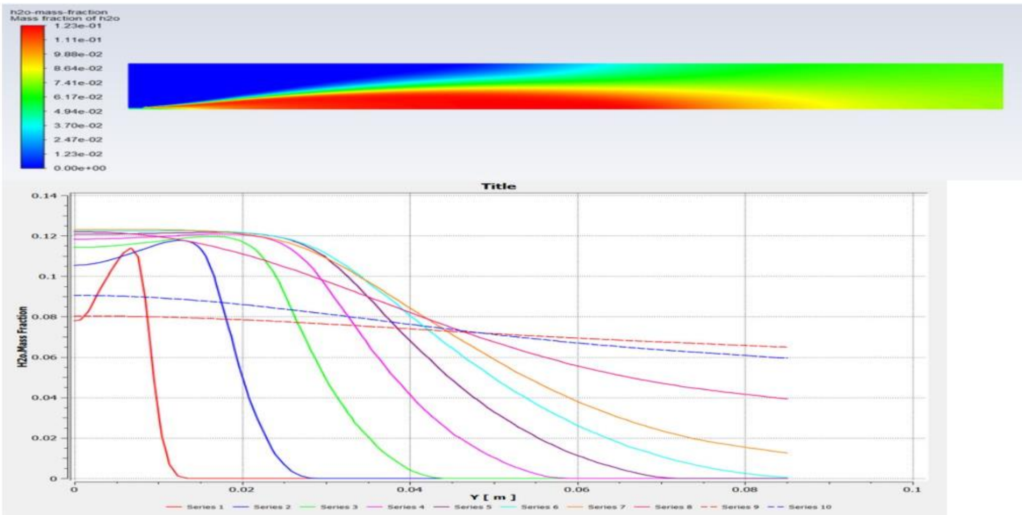
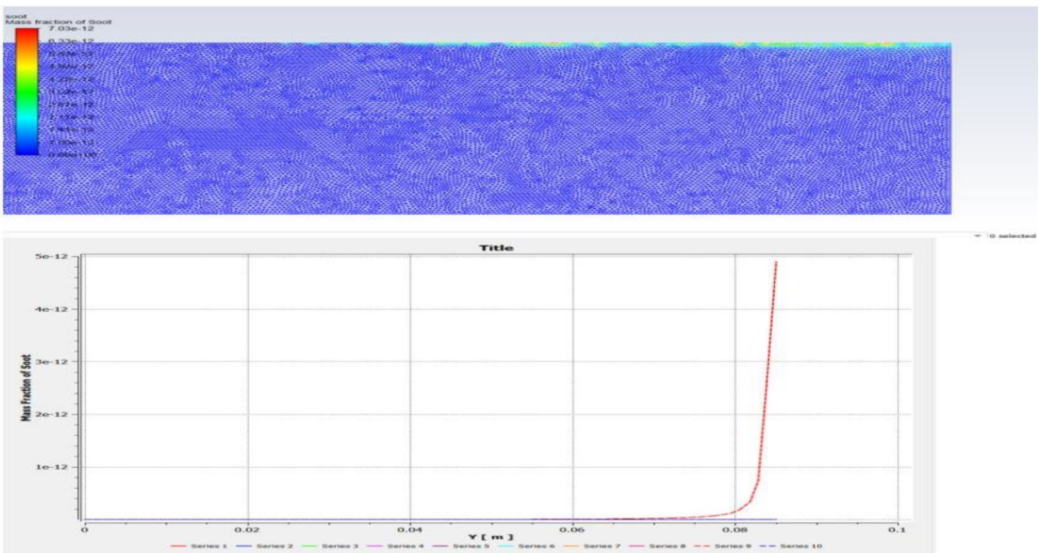
N2O Mass Fraction



H2O Mass Fraction



SHOOT Mass Fraction



8. Conclusions

After all the work done, the results show pretty interesting results. It is clear that the addition of water has a significant effect on the NOx formation. More water is added to the system, less NOx are formed.

Also it leads to increased OH radicals that might have a significant impact in SOOT Oxidation and reduce the SOOT formed in Gas Phase. If temperature reduces sufficiently, NOx cannot form in great concentration.

This work gives the tendency of the NOx formation when adding water to the system, but the reaction mechanism, the radiation model and other system' parameters used for the simulations are quite simple, so the results must be taken, as this is, a tendency.

9. Future Scope

It would be very interesting to compare the simulations with an experimental assay to validate the models used in the study.

However, one must this work implies much more time than is available for a master thesis, e.g. a PhD would be required. System selection and apparatus montage, and detailed modeling and calculations implies lots of time, but would be worth spending if these studies carry innovation and solutions for the problematic issue of NOx pollution.

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