



**GINA CODY SCHOOL OF ENGINEERING AND COMPUTER
SCIENCES**

**DEPARTMENT OF MECHANICAL, INDUSTRIAL AND AEROSPACE
ENGINEERING**

FINAL PROJECT REPORT

MECH 6191 Low Emissions Combustion Design Case Study

SUBMITTED BY

ADHEESH TIRUPATHIPANNYA SANJAY – 40196134

DHYAN RAJESHKUMAR THAKER – 40203663

BHAVIK BAROT – 40234381

NILAY CHAVDA – 40239119

SUBMITTED TO

Dr. PIERRE GAUTHIER

Abstract:

This project focuses on the design and analysis of a hydrogen-fuelled fuel injector with the primary objective of minimizing NO_x emissions. The design process incorporates state-of-the-art technologies and engineering principles to optimize injector performance. The design parameters are defined and implemented, leveraging advanced computational tools like ANSYS Fluent for comprehensive analysis.

Key aspects of the project include:

Design Criteria: Establishing specific design parameters based on the operational requirements and characteristics of hydrogen combustion within gas turbines.

Technology Integration: Incorporating cutting-edge injector technologies to enhance efficiency and combustion characteristics while reducing emissions.

Simulation and Analysis: Utilizing ANSYS Fluent for computational fluid dynamics (CFD) simulations to evaluate the performance of the injector design, particularly focusing on NO_x emissions.

Performance Evaluation: Comparing actual performance against theoretical calculations to identify areas for improvement.

Iterative Design Process: Iteratively refining the injector design based on simulation results and performance evaluations to achieve optimal efficiency and reduced NO_x emissions.

The outcome of this project aims to contribute towards the development of cleaner and more efficient gas turbine technologies by providing insights into the design and optimization of hydrogen fuel injectors.

Table of contents.....	3
List of tables	3
1. Introduction:.....	5
2. Literature survey:	6
2.1 Hydrogen combustion:.....	6
2.2 Combustion control parameters:	7
2.3 Types of NOx:.....	7
2.4 Other options of sustainable fuels:	7
3. Project objectives:	8
4. Modelling parameters:	8
4.1 Turbulence Model:.....	8
4.2 NOx modelling:	9
4.3 PDF mixture:.....	9
4.4 Non-Premix combustion model:	9
4.5 Radiation P1 model:.....	10
4.6 Sutherland Viscosity model:	10
5. Stoichiometric & Injector Design Calculation:.....	11
6. Injector Modeling:	16
7. Volumetric Analysis (Combustion Details).....	24
7.1 Results for Model-1 at the equivalence ratio of 0.65	24
7.2 Results for Model-2 at the equivalence ratio of 0.65	27
7.3 Results at design the equivalence ratio of 0.55	34
7.4 Results at design the equivalence ratio of 0.75	38
8. Results and Discussion:	Error! Bookmark not defined.
9. Conclusion:	41
10. References:.....	42

[Table of contents](#)

[List of tables](#)

Table 1 Design parameters for injector design	8
Table 2 Sutherland's Law Parameters for Dynamic Viscosity	11
Table 3 Density and Velocity parameters	12
Table 4 Design parameters for Equivalence Ratio of 0.65	12
Table 5 Flame temperatures at different equivalence ratios	15
Table 6 Simulation parameters for model 1	15
Table 7 Simulation parameters for model 2	15
Table 8 Model 1 design parameters for Injector and combustor	17

Table 9 Model 2 design parameters for Injector and combustor	19
Table 10 Pressure drop at equivalence ratio 0.65	26
Table 11 Pressure drop at equivalence ratio 0.65	34
Table 12 Pressure drop at equivalence ratio 0.55	37
Table 13 Pressure drop at equivalence ratio 0.75	40
Table 14 Model parameters for model 2	23

1. Introduction:

Gas turbines are essential internal combustion engines used both for ground-based electrical power generation and airborne propulsion in aircraft. The key components of a gas turbine include the compressor, combustion chamber, and turbine. The process begins with air being drawn into the inlet duct and passing through the compressor, where its pressure increases significantly. This compressed air is then mixed with fuel and directed into the combustion chamber, where the mixture is ignited, resulting in the generation of hot gases. These high-temperature gases are then directed through the turbine, where their pressure and temperature decrease, ultimately passing through the nozzle to produce thrust or power.

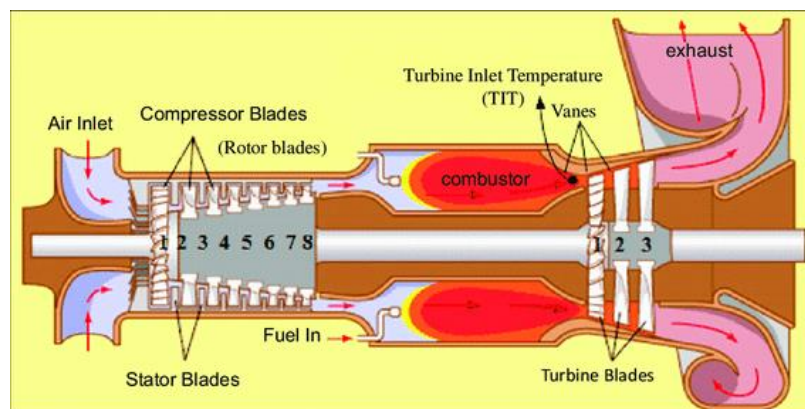


Figure 1 Cutaway of a Gas Turbine (1)

The term "gas turbines" stems from their utilization of gases, typically hydrocarbons, as fuel to rotate components and generate thrust. However, the use of hydrocarbon fuels in gas turbines poses significant environmental challenges, as it contributes to the release of harmful greenhouse gases such as nitrogen oxides (NO_x) and carbon dioxide. Given the escalating concerns surrounding global warming, these emissions play a critical role in addressing environmental sustainability across various industries, including aviation.

The aviation sector represents a notable contributor to global emissions, accounting for approximately 2% of total greenhouse gas emissions. Despite this modest share, the aviation industry faces substantial challenges in mitigating emissions due to its unique operational demands and technological constraints. To combat this, extensive research efforts have focused on identifying sustainable solutions to reduce aviation emissions. A key area of exploration involves the adoption of alternative fuels, such as Sustainable Aviation Fuels (SAF), and investigating the viability of hydrogen as a future aviation fuel.

Hydrogen has emerged as a promising candidate for decarbonizing aviation, offering the potential to significantly reduce greenhouse gas emissions compared to conventional jet fuels. However, transitioning to hydrogen in aviation presents its own set of challenges, spanning from production and storage to combustion and emissions control. One primary concern associated with hydrogen combustion in aviation engines is the tendency for high temperature burning, leading to the formation of nitrogen oxides (NO_x), which are detrimental to air quality and the environment.

The successful integration of hydrogen as an aviation fuel hinges on addressing these critical challenges, particularly optimizing combustion processes to strike a balance between efficient energy release and controlled emissions. Effective temperature management is crucial to mitigate

excessive NO_x formation while ensuring complete combustion of hydrogen. This intricate balance underscores the complexity of integrating hydrogen into aviation propulsion systems and emphasizes the need for innovative engineering solutions and rigorous scientific inquiry to pave the way for a sustainable future in aviation.

2. Literature survey:

The study demonstrates the efficacy of employing the micromix concept in combustors to enhance mixing efficiency and broaden the flammability range of hydrogen-air flames compared to traditional kerosene combustors. The research highlights that the improved mixing capability allows the combustion zone to operate at significantly lower equivalence ratios, which is critical for achieving stable and efficient combustion of hydrogen. Two distinct models were investigated: Model A, featuring four hydrogen injection holes, and Model B, incorporating two hydrogen and two air injection holes. The introduction of air through two injection holes and hydrogen through the other two within the main flow effectively reduces the extent of high-temperature zones. Specifically, the modified Model B not only decreases NO_x emissions but also achieves a 50% reduction in the length of the combustion chamber compared to conventional designs. This innovative approach holds promise for optimizing hydrogen combustion in gas turbine combustors, contributing to cleaner and more efficient aviation propulsion systems. [1]

This paper explores four design variations derived from key parameters using numerical simulations. Findings indicate that optimizing jet penetration can reduce NO_x emissions under higher global equivalence ratios. Additionally, variations in air gate geometry significantly influence flame shape, highlighting the potential to alter flame characteristics with different designs while maintaining a constant momentum flux ratio. [2]

The study proposes a novel solution for improving scramjet performance through a strut fuel injector featuring a wavy wall surface and multiple struts, compared to a single wedge design using computational simulations. Results show significant benefits with the wavy-wall double strut, including increased mixing efficiency and combustion phenomena, resulting in an 18% boost in mixing efficiency and 20% improvement in combustion efficiency. The revised strut design offers potential advantages such as a shorter combustor length, lower drag force, and higher downstream turbulence intensity. [3]

The authors discuss challenges in lean premixed system design, particularly flame flashback into the burner, weighing the trade-off between increased burner velocities and higher-pressure drop. The study emphasizes the risks of flame flashback with rising firing temperatures to maximize efficiency. Special attention is given to hydrogen's flammability limits and laminar flame speed, alongside investigations into flashback mechanisms, combustion instabilities, and turbulent flame speed. The review delves into combustion-induced vortex breakdown (CIVB) in swirling flames, exploring heat release, vortex aerodynamics, and flame quenching interactions, with a focus on post-flashback flame holding using fuel injection jets, especially in crossflow mode. Insights from supersonic applications and subsonic jet flame holding behavior contribute to a comprehensive overview of current research challenges and complexities in lean premixed combustion. [4]

2.1 Hydrogen combustion:

As mentioned earlier, hydrogen presents itself as a promising alternative to hydrocarbons, but several challenges must be addressed. Firstly, the production of hydrogen often involves significant

carbon dioxide emissions, which is a drawback for its environmental impact. Additionally, storing hydrogen is a major concern due to its highly flammable nature and the requirement for cryogenic temperatures (around -253 degrees Celsius) to maintain its liquid state. This necessitates large, specialized containers that are cumbersome and not easily transportable.[5]

Furthermore, when hydrogen is used as a fuel or additive, the primary concern is flashback due to its high burning velocity compared to natural gas. This poses a critical issue for many domestic combustion devices that use premixing techniques. Flashback can result in equipment damage or flame extinction, leading to the release of combustible mixtures into living spaces, thereby endangering end users' safety. These challenges highlight the need for innovative solutions in hydrogen production, storage, and utilization to fully realize its potential as a cleaner energy source. [6]

2.2 Combustion control parameters:

When burning hydrogen, critical factors to consider include flame speed and flame temperatures. Hydrogen has a significantly higher flame velocity compared to other gases thus it must be under control to prevent flashback during combustion. To mitigate this risk, the hydrogen fuel velocity must be carefully managed to ensure it remains in controlled levels. Additionally, high hydrogen flame temperatures can lead to increased NO_x formation, highlighting the importance of temperature control to minimize environmental impact. These considerations underscore the complexity of optimizing hydrogen combustion for efficiency and emissions control in various applications.

2.3 Types of NO_x:

Thermal NO_x formation is strongly reliant on temperature, pressure, and residence time, hence reducing factors leads to lesser NO_x production. Thermal NO_x generation rates are minimal in current combustion devices. Fuel NO_x is the byproduct of the fuel's nitrogen reacting with oxygen during combustion. While liquid fuels with a high nitrogen content cause more NO_x emissions, gaseous fuels present less problems. Prompt NO_x may form because of air nitrogen reacting with combustion radicals; it can also form independently of fuel and thermal NO_x. There is no temperature dependence in prompt NO_x emissions.

2.4 Other options of sustainable fuels:

There are other blends of alternative fuels such as Bio-Jet fuels, Electro-Jet fuels, Ammonia etc. Various alternative aviation fuels are being explored to reduce emissions and enhance sustainability. Bio-jet fuels offer low exhaust toxicity when blended with conventional jet fuel, with similar energy content and properties for compatibility with existing engines. Electro-jet fuels, derived from electricity through water electrolysis with captured carbon or nitrogen, present diverse options like Fischer-Tropsch kerosene, methane, and hydrogen. Liquefied methane (LNG) shows promise but faces challenges in infrastructure and tank design due to its cryogenic storage requirements like Hydrogen. Ammonia is considered due to its high hydrogen content and potential use in modified aircraft engines and fuel cells, offering flexibility in low-blend or dual-fuel applications. Each of these alternative fuels presents unique opportunities and challenges for advancing sustainable aviation. [7]

3. Project objectives:

The main objectives of this project are

- 1- Design 2 fuel injectors for Hydrogen combustion Gas Turbines which can produce low NO_x.
- 2- Calculate stoichiometric calculations such as FAR, velocity of fuel.
- 3- Perform ANSYS Fluent analysis for NO_x calculations.

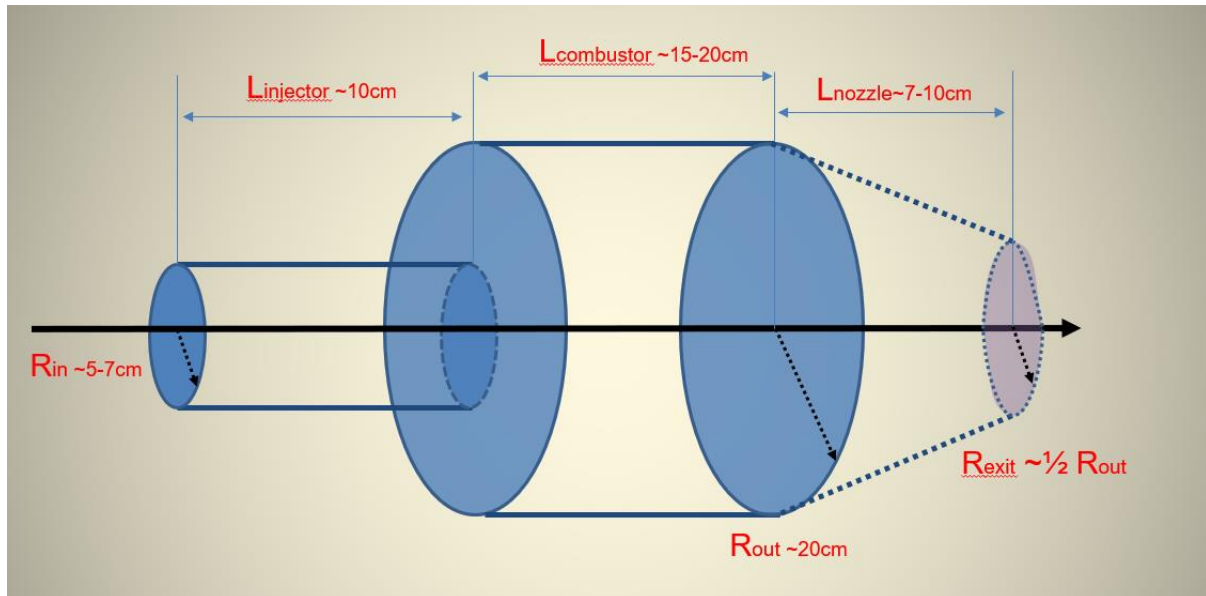


Figure 2 Injector and Combustor design parameters

DESIGN PARAMETERS	
Temperature of air at inlet	700 K
Temperature of fuel	300 K
Air density at 700 K, 15 bar	5.3697 kg/m ³
Hydrogen density at 300 K, 15 bar	1.2124 kg/m ³
Outlet temperature	1500 K

Table 1 Design parameters for injector design

The fuel injectors are designed with these parameters in mind.

4. Modelling parameters:

4.1 Turbulence Model:

We have used $k-\epsilon$ Realizable model for turbulence in our setup. The realizable $k-\epsilon$ model is a recent development and differs from the standard k -model in two important ways:

- The realizable $k-\epsilon$ model contains a new formulation for the turbulent viscosity.

- A new transport equation for the dissipation rate has been derived from an exact equation for the transport of the mean-square vorticity fluctuation.

The term “realizable” means that the model satisfies certain mathematical constraints on the Reynolds stresses, consistent with the physics of turbulent flows. Neither the standard k-model nor the RNG k-model is realizable.

An immediate benefit of the realizable k-model is that it more accurately predicts the spreading rate of both planar and round jets. It is also likely to provide superior performance for flows involving rotation, boundary layers under strong adverse pressure gradients, separation, and recirculation.

4.2 NO_x modelling:

Thermal NO_x modelling is considered in Model 1. Thermal NO_x - a reaction between oxygen and nitrogen in the combustion air at temperatures >1300°C in oxidising atmospheres; dependent on flame temperature and residence time at high temperatures; predominantly formed in the flame envelope.

Thermal NO_x is produced via a series of oxidation reactions, known as the ‘Zeldovich mechanism’. This is shown in equations 1 and 2.



In a fuel-rich environment, the reactions change slightly as follows:



$$0.55 = 0.00046427446$$

$$0.65 = 0.00050484634$$

$$0.75 = 0.0018061499$$

4.3 PDF mixture:

PDF mixture modelling, an integral component of Ansys Fluent, which changes the simulation of turbulent reacting flows by employing probability density functions (PDFs) to represent flow variables like species concentrations and temperature distributions. By embracing the inherent complexity of turbulent flows and utilizing concepts such as mixture fraction, PDF mixture modelling accurately captures turbulent mixing processes critical for understanding phenomena like combustion and chemical reactions. Leveraging probability density functions, it provides a detailed statistical representation of flow variables, enabling accurate modelling of turbulent mixing processes inherent in phenomena like combustion and chemical reactions.

4.4 Non-Premix combustion model:

In non-premixed combustion, fuel and oxidizer enter the reaction zone separately, unlike premixed systems where they are thoroughly mixed before combustion at the molecular level. Examples of

non-premixed combustion scenarios include pulverized coal furnaces, diesel internal-combustion engines, and pool fires.

Under certain simplifications, the thermochemistry involved can be represented by a single parameter known as the mixture fraction, denoted as 'f'. This parameter represents the mass fraction originating from the fuel stream, indicating the local mass fraction of both burnt and unburnt fuel stream elements (such as C, H, etc.) within all species present (such as CO₂, H₂O, O₂, etc.). This approach is elegant as it conserves atomic elements in chemical reactions, making the mixture fraction a conserved scalar quantity. Consequently, its transport equation does not include a source term. This simplifies combustion to a mixing problem, avoiding complexities associated with closing nonlinear mean reaction rates. Once mixed, the chemistry can be further modeled as being in chemical equilibrium using the Equilibrium model, approaching chemical equilibrium with the Steady Laminar Flamelet model, or deviating significantly from chemical equilibrium using the Unsteady Laminar Flamelet model. [9]

The non-premixed combustion model uses a method termed mixture fractions to solve transport equations for one or two conserved scalars. This method makes it possible to include different chemical species in the model, including radicals and intermediate species. The anticipated distribution of mixture fractions is used to calculate the concentrations of these species. [8]

4.5 Radiation P1 model:

The P-1 radiation model represents the most basic form of the broader P-N model. It is derived from expanding the radiation intensity, denoted as 'I', into an orthogonal series of spherical harmonics.[10]

Boundary Condition Treatment for the P-1 Model at Walls is defined as

$$q_{r,w} = -\frac{\epsilon_w}{2(2 - \epsilon_w)} (4\pi^2 \sigma T_w^4 - G_w)$$

Figure 3 P1 model boundary condition treatment

4.6 Sutherland Viscosity model:

Sutherland's law, also known as Sutherland's formula, provides an approximation of how gas viscosity changes with temperature, relying on an idealized representation of intermolecular force interactions.

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + S_\mu}{T + S_\mu}$$

Figure 4 Sutherland formula

where S_μ is an effective temperature called the Sutherland constant. Each gas has its own Sutherland constant. [8]

GAS	μ_0	T ₀	S _{μ}
H ₂	$8.411 \cdot 10^{-5}$	273	97

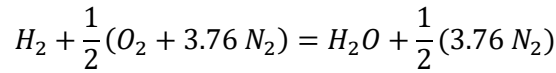
Table 2 Sutherland's Law Parameters for Dynamic Viscosity

5. Stoichiometric & Injector Design Calculation:

We first manually calculated our projected fuel to air ratios and adiabatic flame temperatures at various equivalency ratios to provide us with a starting point for the simulation analysis.

All the calculations were performed here with assumption of Ideal gas law and flame is Non-Premixed Diffusion flame.

1. Stoichiometric Reaction:



Fuel Air Ratio: F/A ratio is an important parameter in designing Injector as it gives value of mass flow rate that is injecting through Air and Fuel hole respectively.

$$\left(\frac{F}{A}\right)_{Stoich} = \frac{\text{mass of fuel}}{\text{mass of oxidizer}}$$

$$\left(\frac{F}{A}\right)_{Stoich} = \frac{2 \cdot 1.00797}{(0.5 \cdot (16 \cdot 2 + 3.76 \cdot 2 \cdot 14))} = 0.028$$

Although combustion characteristics are predicted by equivalence ratio(ϕ) which indicates how lean or rich the fuel in the defined mixture.

$$\phi = \frac{\left(\frac{F}{A}\right)_{Act}}{\left(\frac{F}{A}\right)_{Stoich}}$$

Our aim is to have a fuel lean combustion to help minimize NOx emissions which can be achieved by lowering the equivalence ratio. Hydrogen has a lower flammability limit (Φ) of around 0.1 thus, to be cautious and ensure combustion takes place, we will perform our initial analysis and simulation at an equivalence ratio of 0.65. This gives us our fuel to air ratio for the desired mixture to be:

$$\left(\frac{F}{A}\right)_{Act} = \left(\frac{F}{A}\right)_{Stoich} * \phi$$

Also, we will compare both design with different equivalence ratio of 0.55 and 0.75 to check how does it affect the combustion characteristics i.e. flame temperature and NOx level.

Since we are trying to design cross flow Injection system in which Air and Fuel reacts at 90° . With being noted an important non-dimensional parameter that we must keep in mind is Momentum flux ratio(J).

Finding the input fuel and air velocities was the next stage in estimating the mass flow rate of the fuel and air. This was accomplished by examining our mixture's momentum flux ratio (J):

$$J = \frac{P_{fuel} V_{fuel}^2}{P_{Air} V_{Air}^2} \cong (8 \text{ to } 10)$$

While velocity distribution in case of diffusion flame is best described by its momentum and by maintaining this ratio in the range, we got following values of velocity throughout the injector and combustor.

	Hydrogen (300K)	Air (700K)
Density at 15 bar	1.225	7.465
Velocity (m/sec)	522	80

Table 3 Density and Velocity parameters

By determining values of densities from experimental data((Xiaoxiao Sun, 2020)), fluid velocities should be in such range that meet the minimum criteria for Momentum flux ratio from Literature review. From design data we have Air velocity that is coming out from compressor around 80 m/sec. To maintain momentum flux ratio in given range and allow better mixing. The fuel Inlet velocity is found to be 522 m/sec to obtain momentum flux ratio of 9.

$$J = \frac{1.2 * (V_f)^2}{7.465 * (100)^2}$$

From that we can calculate mass flow rate of fuel by momentum equation.

$$m_f = \rho_f v_f A_f$$

Where m_f can be calculated using F/A ratio explained above.

As mentioned above, that geometry of the fuel and air injector is went through multiple iterations based on the results achieved from the cold flow simulations. From using above equations, we were able to calculate mass flow rates and the dimension of fuel and air hole diameter.

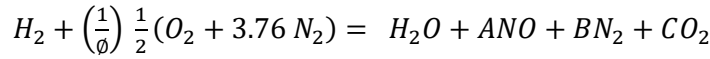
Design for Equivalence Ratio of 0.65	
Area of Air Inlet	1.9625 e-4
Diameter of Air Inlet	0.00322
Mass flow of Air (kg/sec)	4.68 kg/sec
Mass Flow rate of Fuel (Kg/sec)	0.0088218 kg/sec
F/A Ratio (Stoich)	0.028
Total Fuel Area	9.802 e-5
No of Fuel Inlet	12

Table 4 Design parameters for Equivalence Ratio of 0.65

For combustion simulation we first need to calculate Adiabatic Flame Temperature to help us in analysis of Numerical data. Knowing that we were aiming for fuel lean combustion with an equivalence ratio of 0.65.

2. Off- Stoichiometric conditions:

Off- Stoichiometric reaction is given by:



We have used Cantera simulation software to analyse Adiabatic Flame temperature.

Since we can assume that the combustion in the chamber takes place under constant pressure and adiabatic conditions, we can write enthalpy equations in following manner:

$$Q = \sum_P n_i \bar{h}_i(T_P) - \sum_R n_i \bar{h}_i(T_R) = 0$$

$$\sum_P n_i \bar{h}_i(T_a) = \sum_R n_i \bar{h}_i(T_1)$$

Figure 5 Enthalpy equation

Where the sum of the enthalpy of the products at the adiabatic flame temperature (Ta) must be equal to the sum of the enthalpy of the reactants at their initial temperatures (T1). Expanding the above reaction, we can then start calculating the adiabatic flame temperature (Ta).

$$\sum_P n_i [\bar{h}_{f,i}^\circ + (\bar{h}_i(T_a) - \bar{h}_i(298K))] = \sum_R n_i [\bar{h}_{f,i}^\circ + (\bar{h}_i(T_1) - \bar{h}_i(298K))]$$

Figure 6 Adiabatic flame temperature (AFT) formula

Total Heat of Reaction is given by:

$$\Sigma HR = [\bar{h}_{f,i} + (\bar{h}_i(300K) - \bar{h}_i(298))]_{H_2} + 6.27 [\bar{h}_{f,i} + (\bar{h}_i(700K) - \bar{h}_i(298))]_{N_2}$$

$$+ 1.67 [\bar{h}_{f,i} + (\bar{h}_i(700K) - \bar{h}_i(298))]_{O_2}$$

Figure 7 Total heat of reaction

We have computed Adiabatic Flame temperature with the help of Cantera simulation. Cantera takes all the fundamental values of Enthalpy and entropy from Detailed Chemical Mechanism file. Cantera has inbuilt function call “equilibrium” which calculates Heat of Reaction at different guess of temperature and gives the value of Adiabatic Flame Temperature where Heat of Reaction is equated with Right Hand and Left-Hand side of equation.

Following computation code shows how flame temperature varies with equivalence ratio.

Next figure shows variation of Adiabatic Flame temperature with Equivalence ratio.

```

import cantera as ct
import math
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

[1] ✓ 0.8s Python

gas = ct.Solution('gri30.yaml')
T_adiabatic = []
phi = np.arange(0.5, 2, 0.05)

for i in range(0, len(phi)):
    gas.TP = 300, ct.one_atm
    gas.X = {"H2": 1, "O2": 0.5/phi[i], "N2": 1.57/phi[i]}
    gas.equilibrate("HP")
    T_adiabatic.append(gas.T)
    #print(T_adiabatic, phi)

df_results = pd.DataFrame({'Equivalence Ratio': phi, 'AFT': T_adiabatic})

#print(df_results)

[7] ✓ 0.0s Python

#df_results.to_csv('results_1.csv', index=False)

plt.plot(phi, T_adiabatic, color="pink")
plt.grid()
plt.xlabel(['Equivalence Ratio'])
plt.ylabel(['Temp'])

[8] ✓ 0.1s Python

```

Figure 8 Cantera code for the effect of equivalence ratio on flame temperature

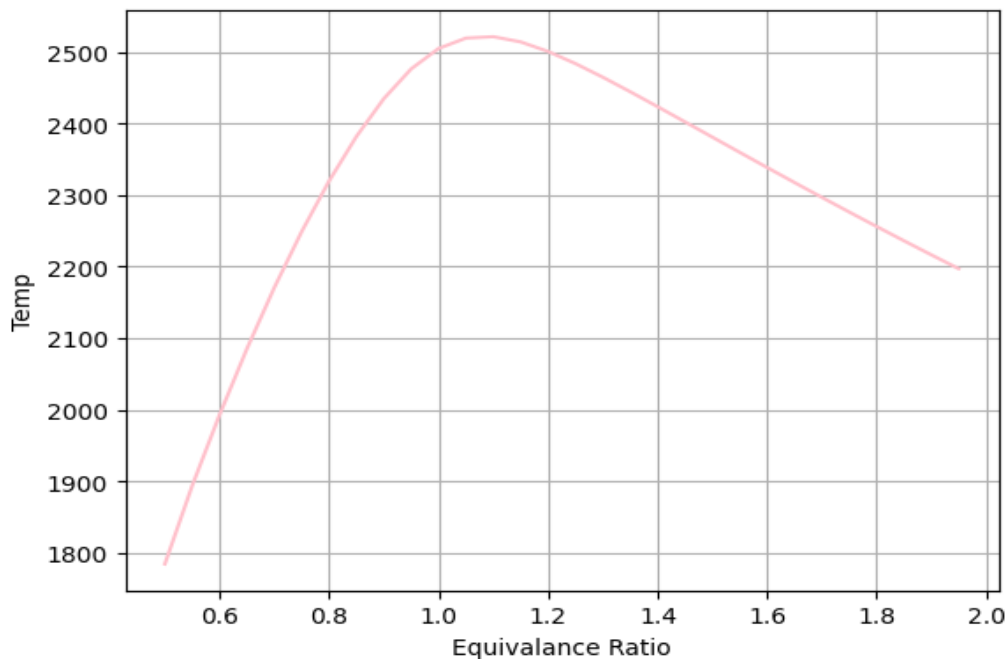


Figure 9 Graph of equivalence ratio vs Adiabatic flame temperature

Assuming that the air and fuel mixture are uniformly distributed throughout the combustor at the intended equivalency ratio ($\Phi = 0.65$), this is the temperature we are trying to reach. We do anticipate some areas in the combustor, though, where the air and fuel mixture were not perfectly premixed, resulting in flame temperatures that are either below or over 1504 K.

We particularly want to stay away from areas where the concentration of fuel is higher than intended because it would result in significantly higher thermal NO_x emissions. To enhance the

identification of these fuel pockets and the level of mixing attained during the combustion simulation analysis, the flame temperatures were computed for various equivalency ratios.

Equivalence Ratio(ϕ)	Adiabatic Flame Temperature (K)
0.5	1784.353
0.55*	1893.913*
0.6	1993.004
0.65*	2085.339*
0.7	2170.753
0.75*	2248.984*
0.8	2319.604
0.85	2381.902
0.9	2434.71
0.95	2476.314
1	2504.812
1.05	2519.339
1.1	2521.337
1.15	2514.029
1.2	2500.701
1.25	2483.753
1.3	2464.699

Table 5 Flame temperatures at different equivalence ratios

Indicates the design points of this project.

3. Values used in simulation:

a. Design-1

Air velocity (m/sec)	80
Fuel Velocity (Hydrogen)(m/sec)	522
Mass flow rate of Air	0.1172 kg/sec
Mass flow rate of Fuel	0.00213218 kg/sec
F/A Stoich	0.028
F/A Actual	0.01885
Equivalence Ratio (ϕ)	0.65
Temperature of Air (K)	700
Temperature of Fuel (K)	300

Table 6 Simulation parameters for model 1

b. Design-2

Air velocity (m/sec)	80
Fuel Velocity (Hydrogen)(m/sec)	522
Mass flow rate of Air	4.68 kg/sec
Mass flow rate of Fuel	0.0088218 kg/sec
F/A Stoich	0.028
F/A Actual	0.01885
Equivalence Ratio (ϕ)	0.65
Temperature of Air (K)	700
Temperature of Fuel (K)	300

Table 7 Simulation parameters for model 2

6. Injector Modeling:

The sole objective of this project is to analyze injector design which aims for low NO_x and has great mixing characteristics with minimum pressure loss across the injector.

Model 1:

We have kept our first model with simple in design and tried to achieve multipoint fuel injection by Injecting fuel with 51 fuel holes with 3.22mm of diameter. Also, we have injected air with 10 air holes with 5mm of diameter circulated in circumferential pattern. Other dimensions like injector length and combustion chamber length were kept as mentioned in the problem statement.

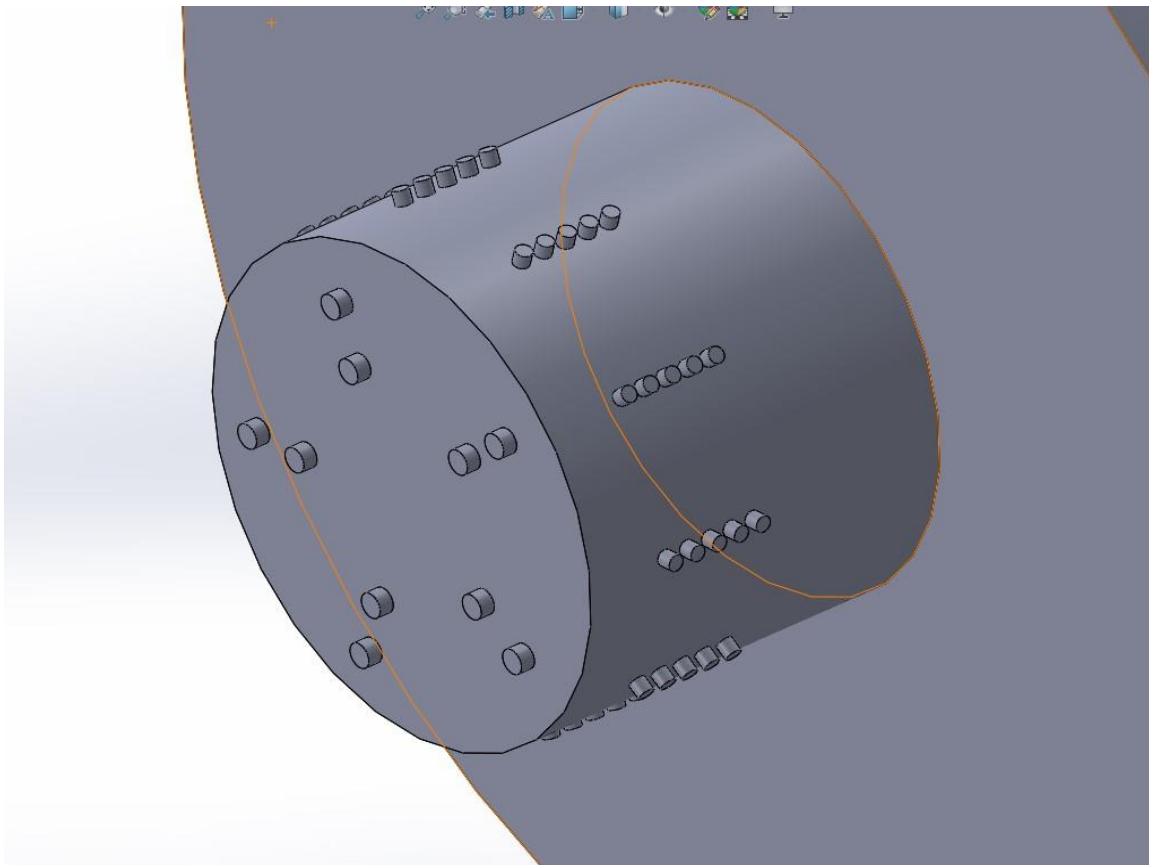


Figure 10 Injector view (Model 1)

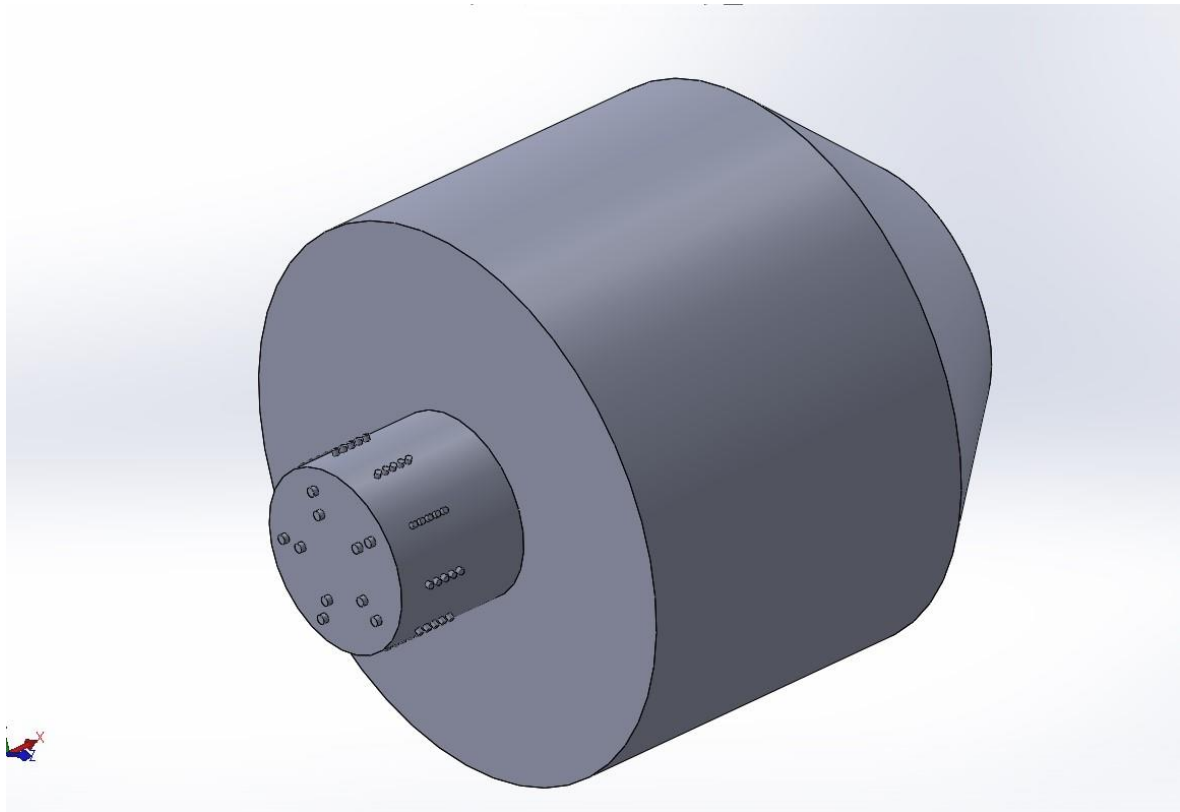


Figure 11 Isometric view (Model 1)

Geometry of Injector and Combustor Design	
Air Inlet Diameter	0.005m
Air Inlet Area	1.9625 e-4
Number of fuel holes	10
Fuel Inlet Diameter	0.0032
Fuel Inlet Area	4.069 e-5
Number of Fuel Holes	10

Table 8 Model 1 design parameters for Injector and combustor

Model 2:

The limitation of the first model is addressed in the second model by introducing swirler. The swirler is mounted in dome of injector circumferentially and plays a key role in combustion design. Swirlers have three basic functions. Firstly, the swirler can create a stable low pressure central recirculation zone that have merits of stabilized and anchored flame close to swirler exit, enhancing mixing between fuel and air and acting as a continuous source of ignition. Secondly, the swirling flow produced by swirler can reinforce the secondary holes recirculation, further increasing the turbulence, which benefits stability of the secondary holes. Finally, the air through the swirler can form a film cooling layer to cool the first section of liner close to the injectors. To fulfil all three functions, the swirler must impart a high radial component, since air which still has an axial component reduces the secondary recirculation. In all, the swirler plays a vital role in gas turbine combustors to improve flame stabilization, fuel air mixing and emissions. (Bhupendra Khandelwal, 2014)

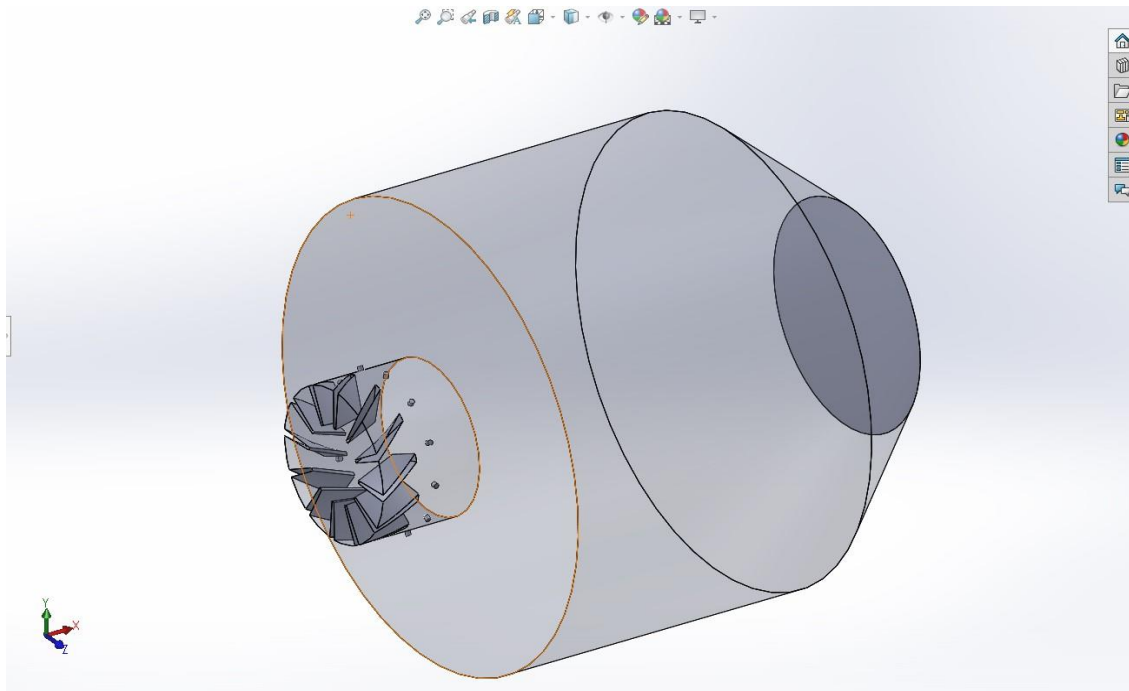


Figure 12 Isometric view (Model 2)

This swirler consists of 12 complex airfoil shaped vanes that are swept for 45° across the surface of Injector. This combination can capture and make swirl of Incoming air and pass it to the combustion process. We have used direct air Inlet to the face of injector and that leads to Inlet diameter of the air is same as Injector diameter.

After swirl action fuel is immediately supplied with 3.22mm diameter of fuel hole and with 12 number of holes circulated on the periphery of the Injector phase. This leads to immediate mixing of fuel and air and results in short flames anchored at the perimeter.

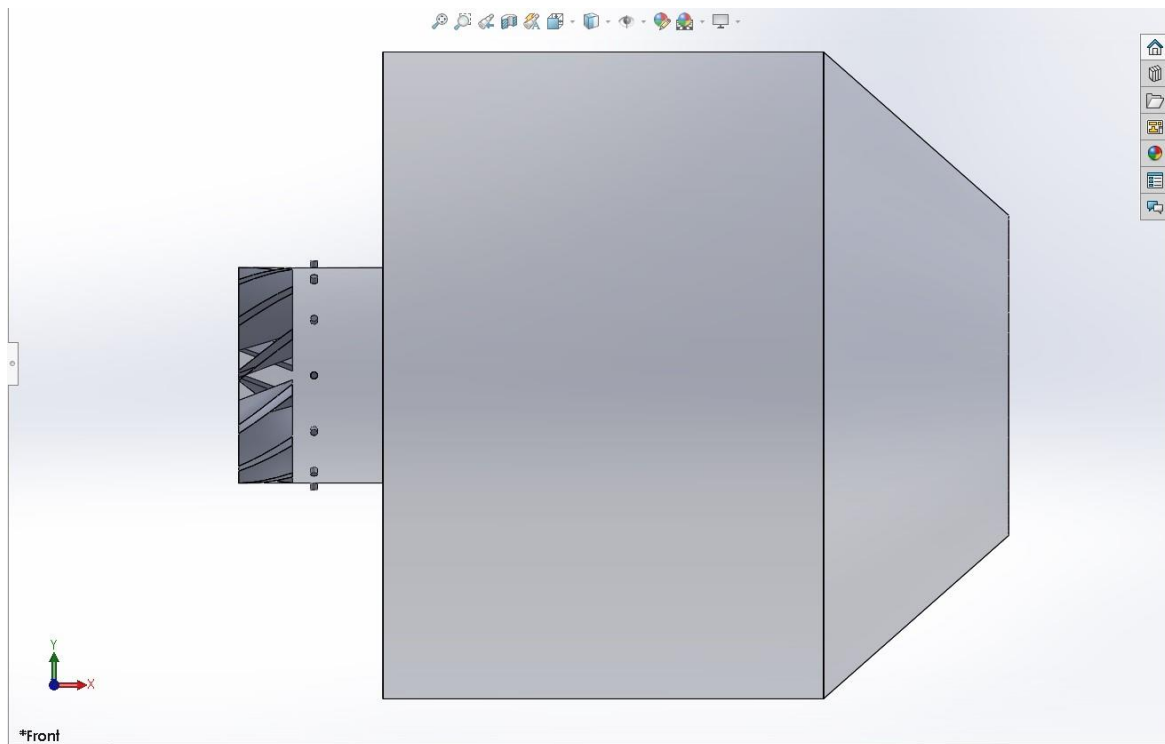


Figure 13. Front view (Model 2)

Dimensions of the Injector and combustor are given in the following table.

Geometry of Injector and Combustor Design	
Air Inlet Diameter (Direct Face Injection)	0.1m
Injector Exit Diameter	0.1m
Air Inlet Area	7.85 e-3
Fuel Inlet Diameter	0.0032
Fuel Inlet Area	9.802 e-5
Number of Fuel Holes	12
Number of Vanes	12

Table 9 Model 2 design parameters for Injector and combustor

The diameter area of the fuel inlets varies with the mass flow rate according to the calculations performed; hence we can update our model and re-run the simulation if required.

7. Results and Discussion:

This analysis takes advantage of the fluent system that ANSYS Workbench employs. SolidWorks geometry is saved as a "step" file, which is imported in the geometry section. Key components, including the guide vanes, fuel and air inlets, combustor output, and walls were defined with the named selection and submitted to meshing.

Model 1:

A linear programmed controlled body mesh is applied to the 3-D model with element size of 7mm. Also face meshing for fuel Inlet is being separately applied with elements size of 1.5 mm to capture the fuel flow behavior effectively. As we know from design data that fuel hole diameter is 3.22 mm which is too small compared to other faces and which requires additional face meshing.

This combination yields a highly refined mesh of 774879 elements and 148252 Nodes (displayed in fig).

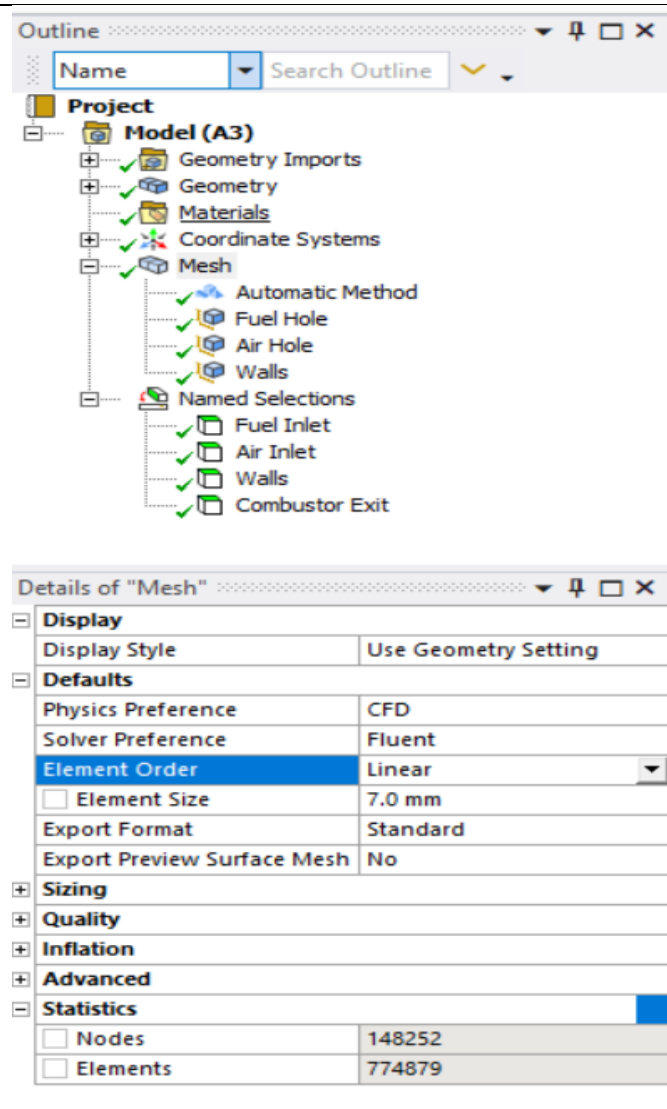


Figure 14. Mesh details (Model 1)

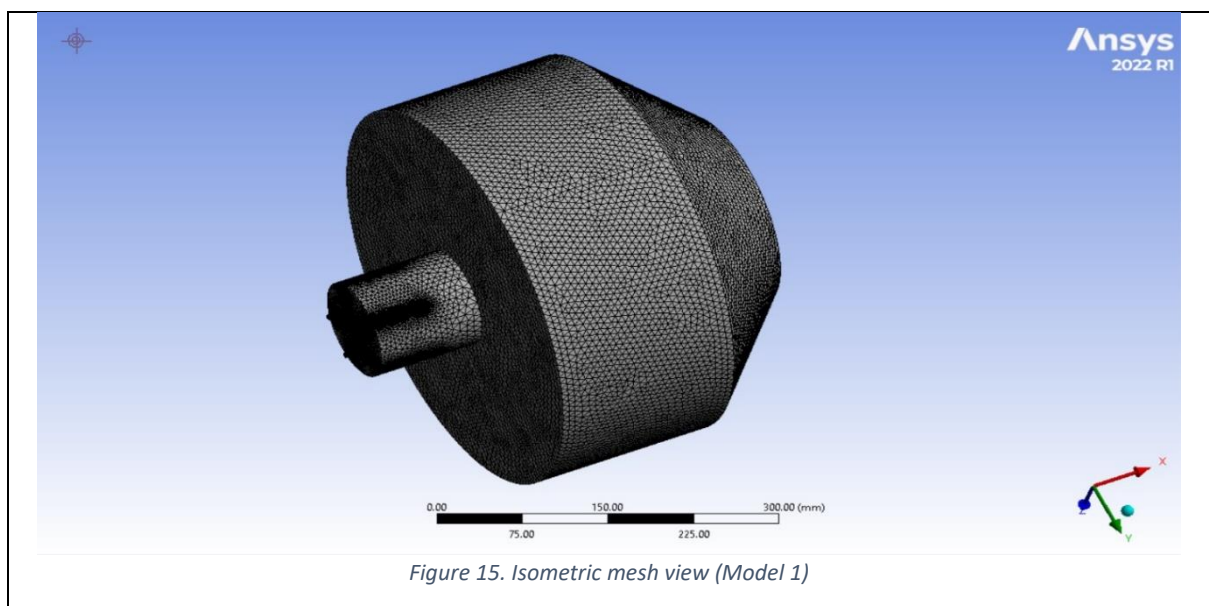


Figure 15. Isometric mesh view (Model 1)

Model 2:

A quadratic programmed controlled body mesh is applied to the 3-D model with element size of 3mm. Also face meshing for fuel Inlet is being separately applied with elements size of 1.5 mm to capture the fuel flow behavior effectively. As we know from design data that fuel hole diameter is 3.22 mm which is too small compared to other faces and which requires additional face meshing.

This combination yields a highly refined mesh of 1445868 elements and 2043393 Nodes (displayed in fig).

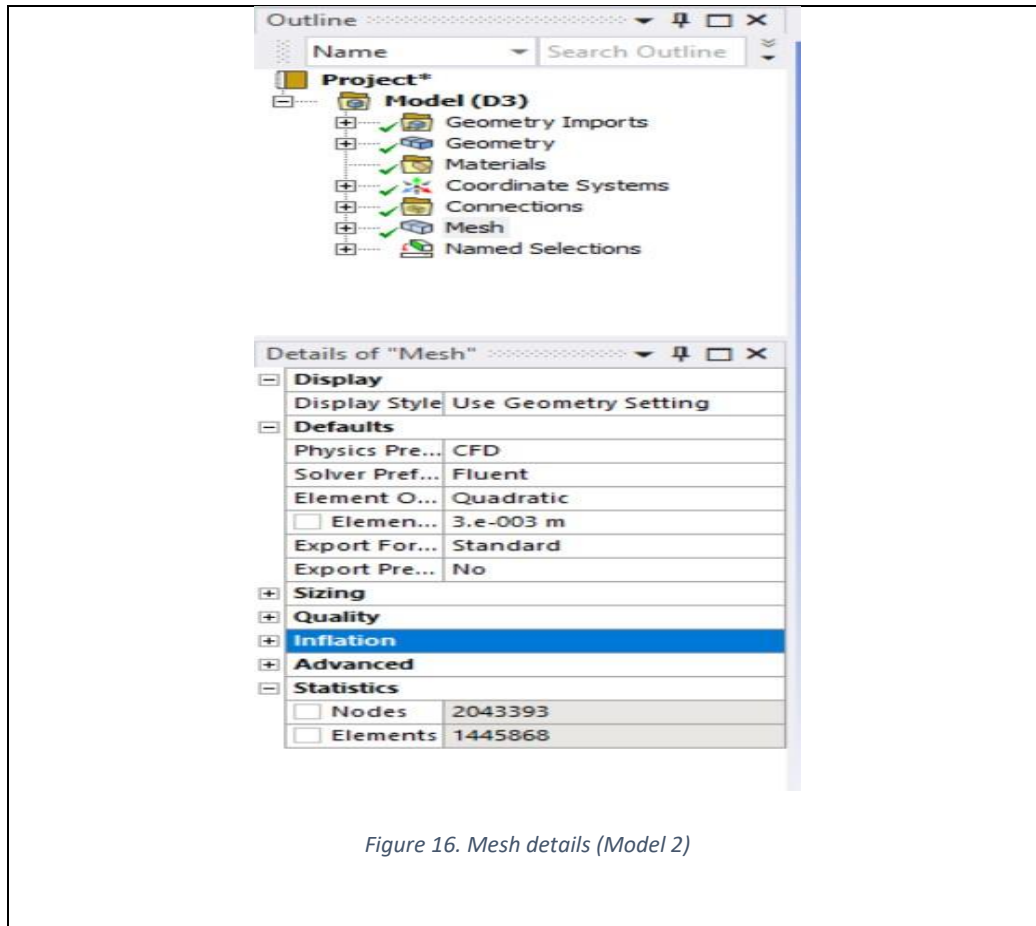


Figure 16. Mesh details (Model 2)

The mesh generated was uniform quadratic with higher mesh concentration at the fuel Inlet. Fig shows the mesh obtained to entire domain.

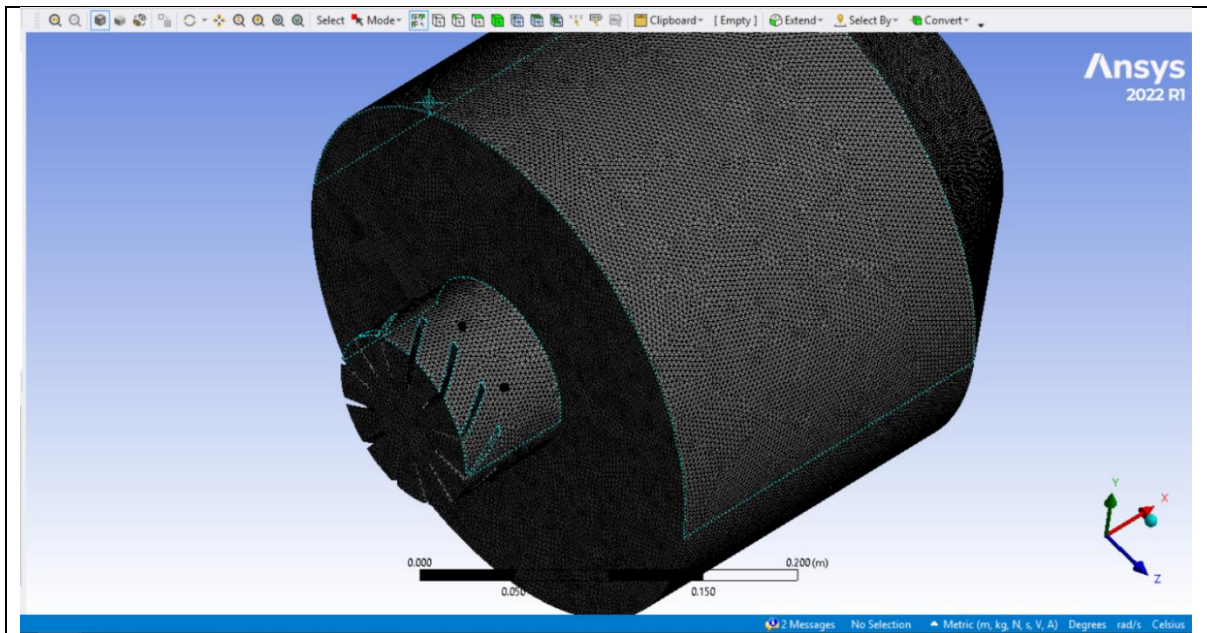


Figure 17. Isometric mesh view (Model 2)

Also, Fig. shows cut section for body meshing to see the mesh quality in the swirl section. It is important to have good quality of mesh in swirl section which leads to capture the fluid flow during recirculation zone.

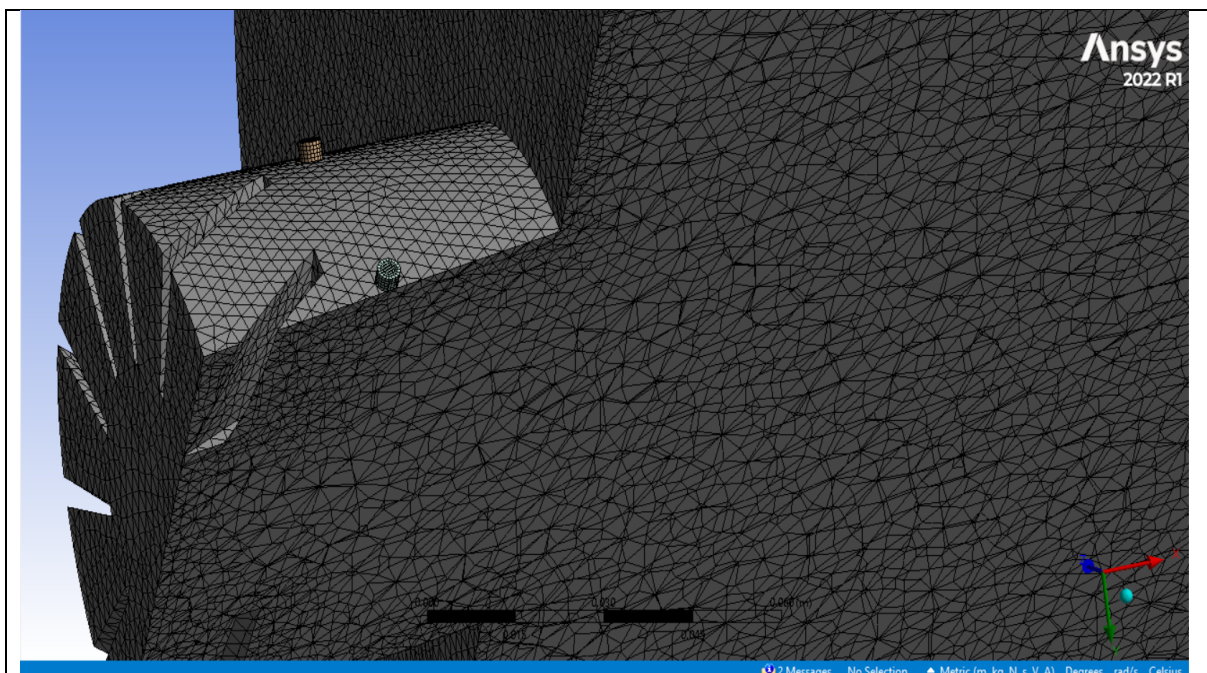


Figure 18. Injector section cut view

The simulation model was then setup using pressure-based solver in steady state analysis. Combustion analysis requires to turn on Energy model to capture flame properties.

All the other modelling parameters have been discussed in above chapter and same setup has been used for initial calculations.

Turbulence Viscosity	k- ϵ
Radiation	P1
Species	Non-Premixed combustion model
Inlet Diffusion (Non Premixed Combustion)	Yes
Fuel Rich Flammability limit (Non-Premixed Combustion)	0.035
Operating Conditions	15.3 MPa
Fuel Inlet Temp (K)	300
Air Inlet Temp (K)	700
Density	Ideal Gas
Viscosity	Sutherland model

Table 10 Model parameters for model 2

k- ϵ Model is usually used for free-shear layer flows when the pressure gradient is relatively small (Acharya, 2016), since our simulation has low pressure drops and less turbulence, the k- ϵ model is the most appropriate choice for our simulation.

As mentioned in table fuel rich flammability limit is an important parameter in flame characteristics. Major reason behind choosing hydrogen as fuel is because of its wide range of flammability limit. Hydrogen has 4 to 74 % by volume of flammability limit i.e. that define flame can sustain over too lean and too rich condition. Multiplying highest flammability with mass fraction and normalizing it gives 0.035 as rich flammability limit.

Density is the function of temperature, and we have wide range of variation of temperature in the combustor so must select density as ideal gas model instead of constant density.

Same applied to viscosity as well, we have to select reliable viscosity model that changes with temperature and take into account. Sutherland's viscosity model is used for viscosity modelling.

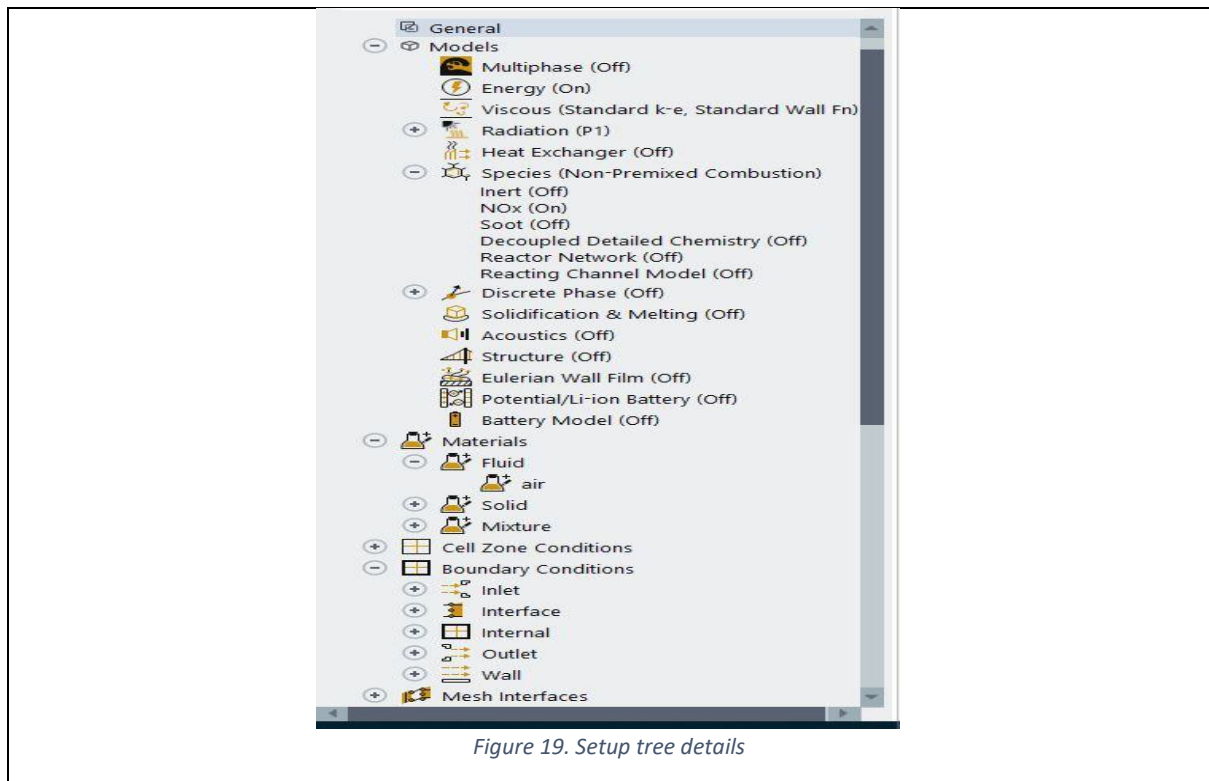


Figure 19. Setup tree details

8. Volumetric Analysis (Combustion Details)

8.1 Results for Model-1 at the equivalence ratio of 0.65

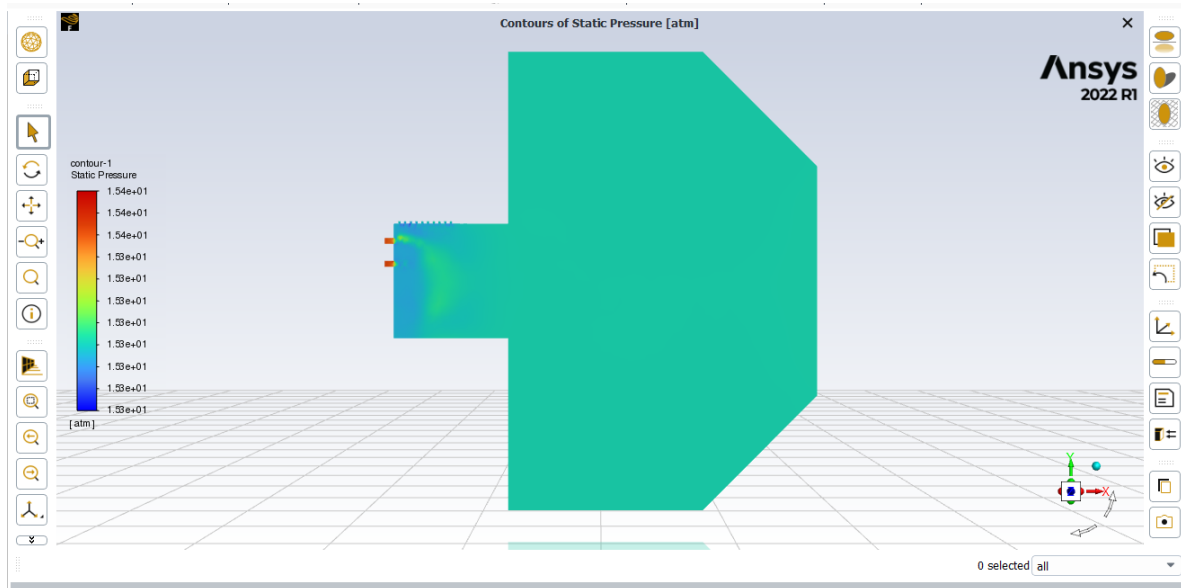


Figure Static pressure contour ($\Phi=0.65$ - Model 1)

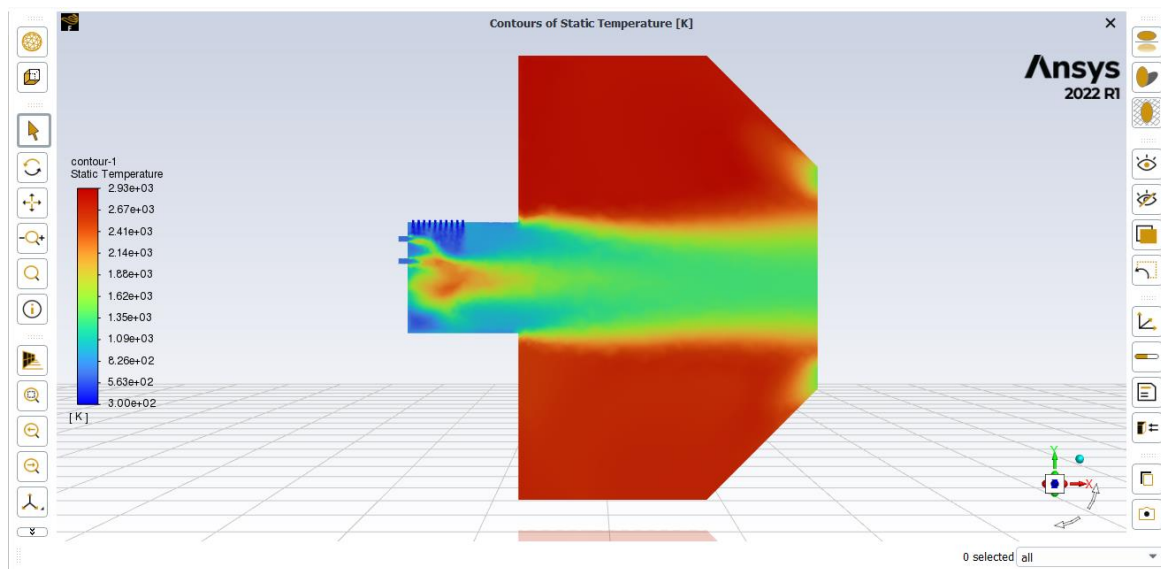


Fig 20 helps us to capture pressure loss occurring during air- fuel contact in the injector. As the velocity decreases during the mixing, decrease in pressure follows as both are directly proportional.

Further, Fig 21 indicates flame propagation over the length of combustor. The reason for central void in the flame is because hydrogen is reactive and even with high velocity, penetration of hydrogen is not achieved at the centre causing the centre of the flame to not react completely with hydrogen.

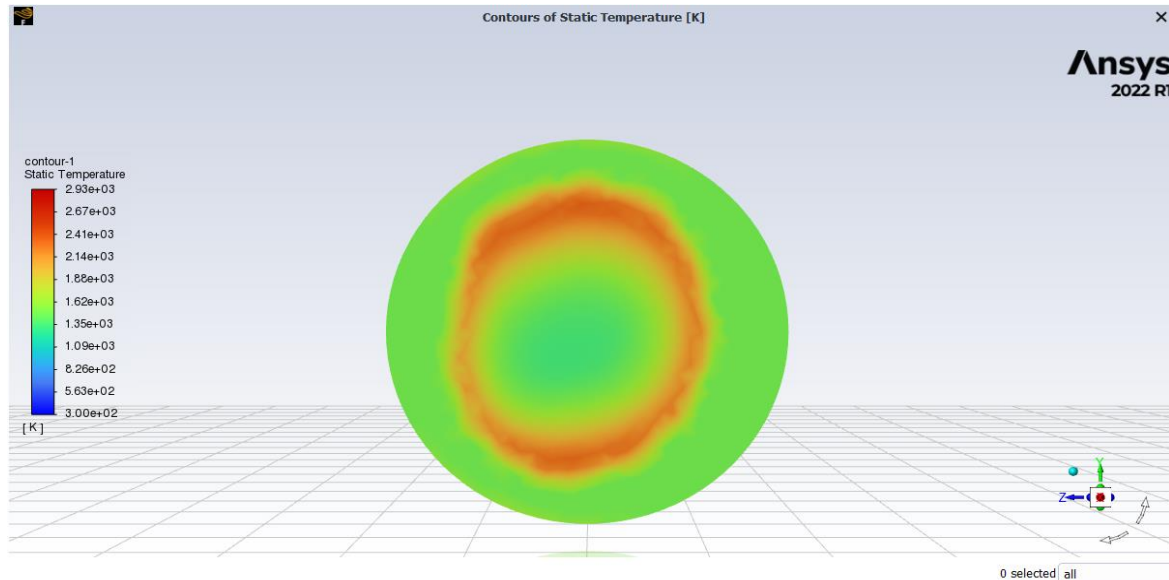


Figure 22. Static temperature at pressure outlet

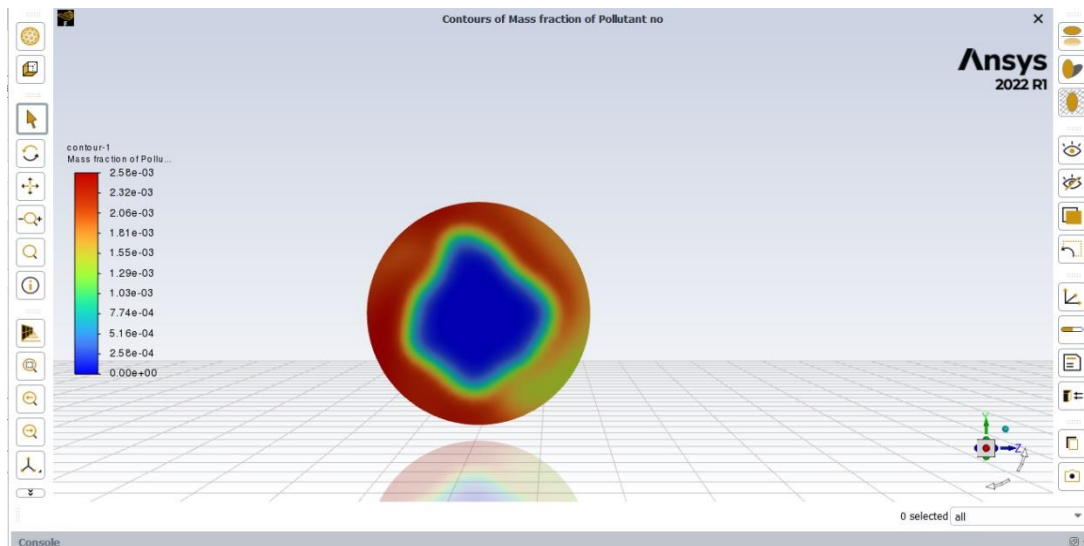


Figure 23. NOx formation at pressure outlet

It is clear from the figure that NO_x formation at the exit of combustion chamber is significant due to improper mixing of fuel and air. In this simple design air is making reaction with fuel at 90 degree and incomplete combustion take place due to high velocity of air.

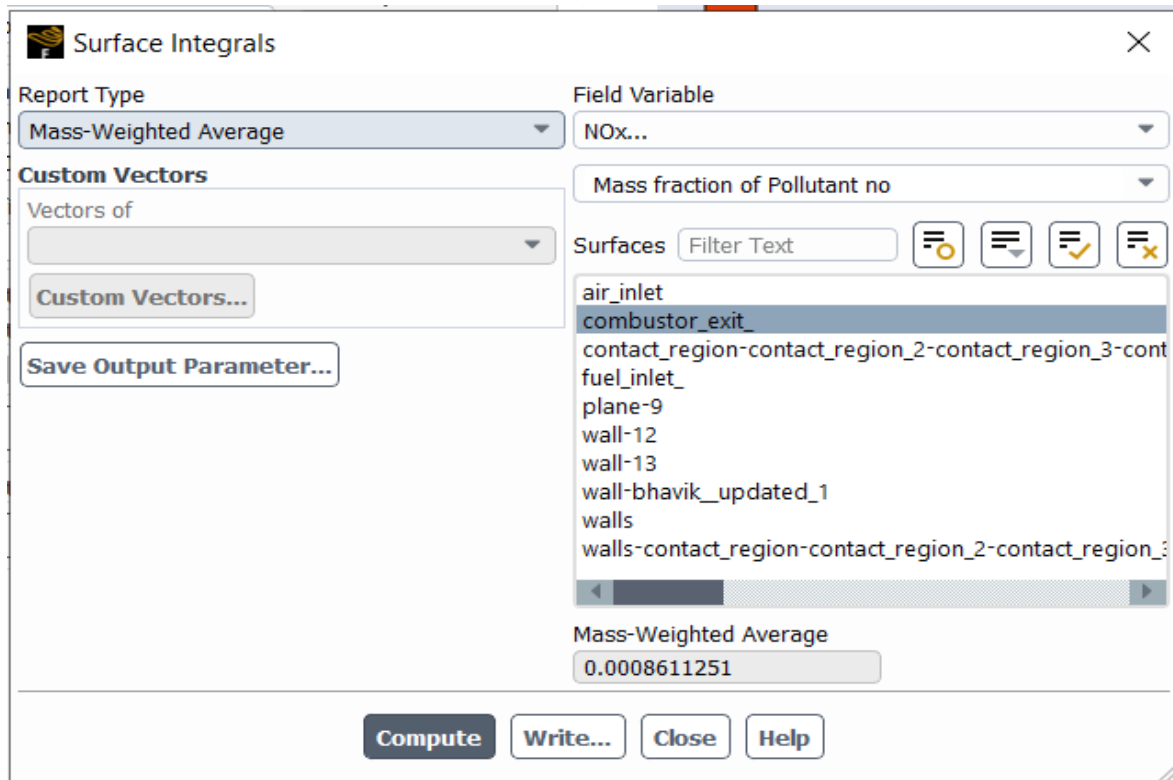


Figure 24. Mass-weighted average concentration of NO_x at pressure outlet

Results for Model-1 at an Equivalence ratio of 0.65

Pressure drops across the Injector	5%
Outlet Temperature	2200 K (Considering flame only)
Nox	861 PPM

Table 11 Pressure drop at equivalence ratio 0.65

8.2 Results for Model-2 at the equivalence ratio of 0.65

The residuals are shown here. We can see that combustion simulation continuing with 2000 iterations and still one of the components of continuity equation is not fully converged.

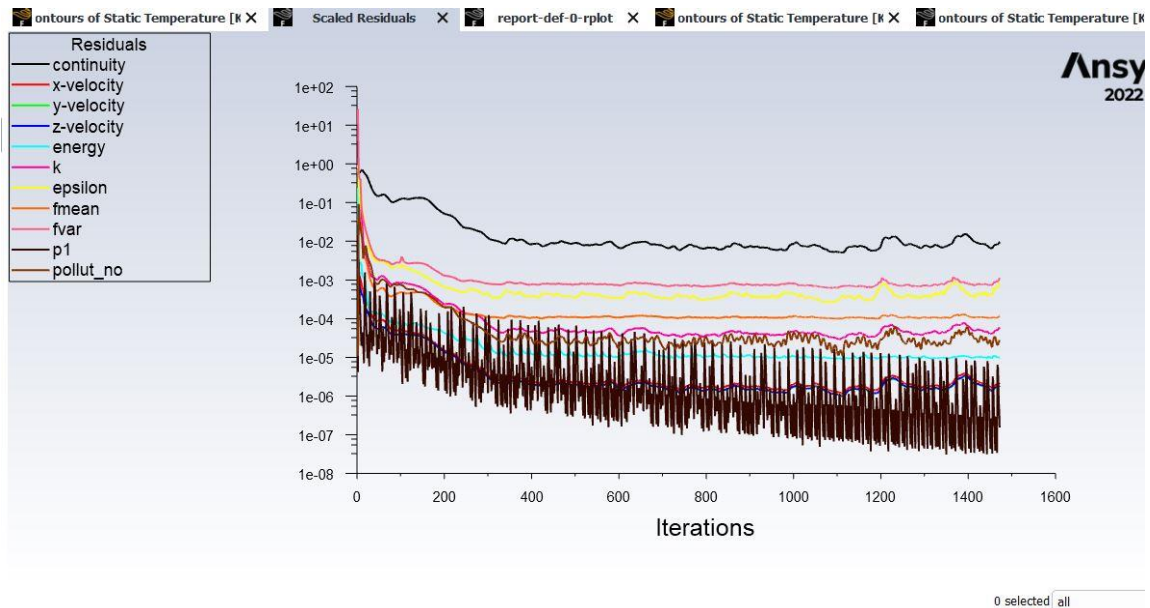


Figure 25. Residual plot (Model 2)

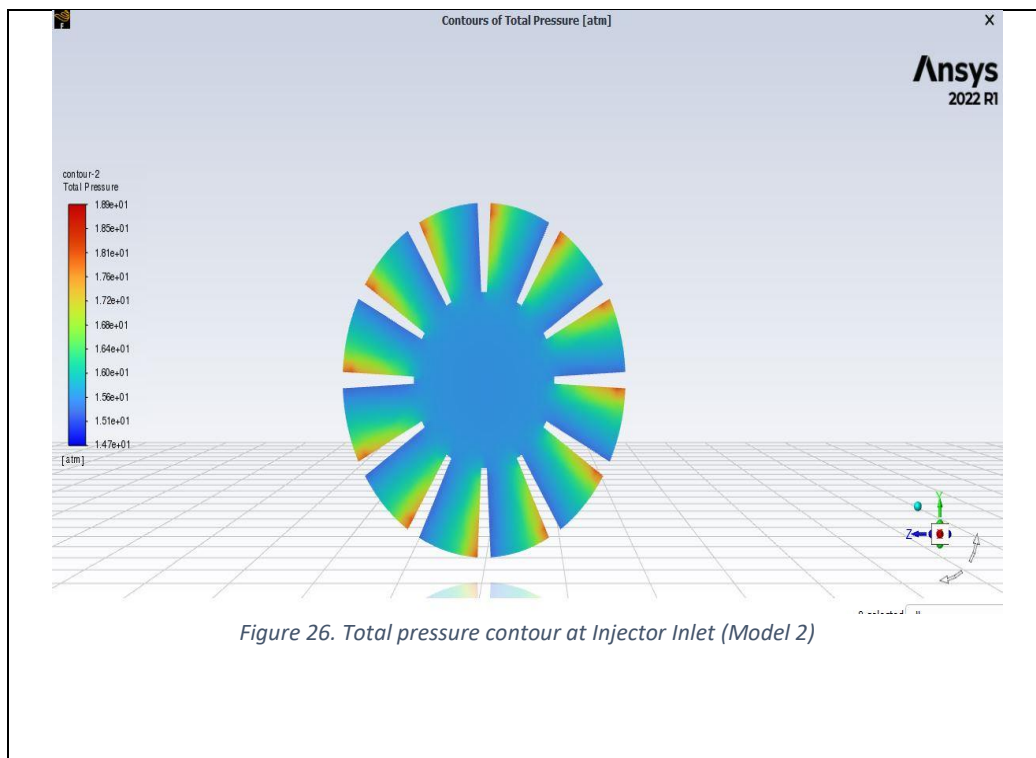


Figure 26. Total pressure contour at Injector Inlet (Model 2)

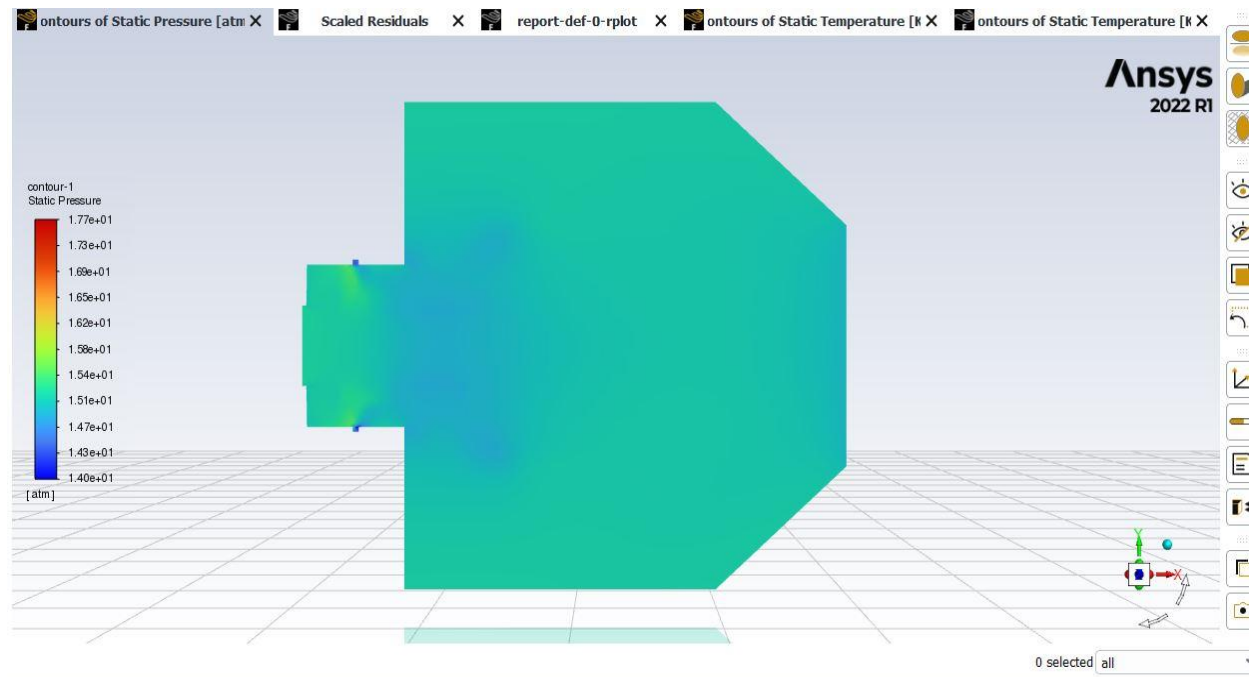
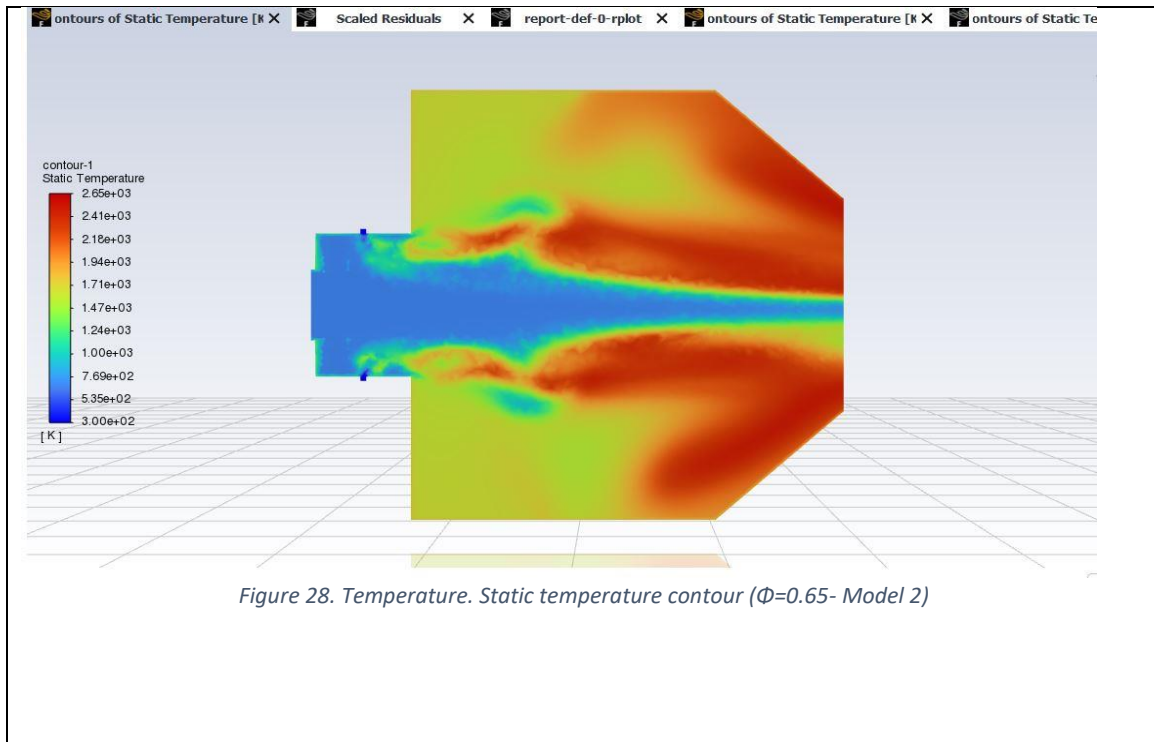


Figure 27. Static pressure contour ($\Phi=0.65$ - Model 2)

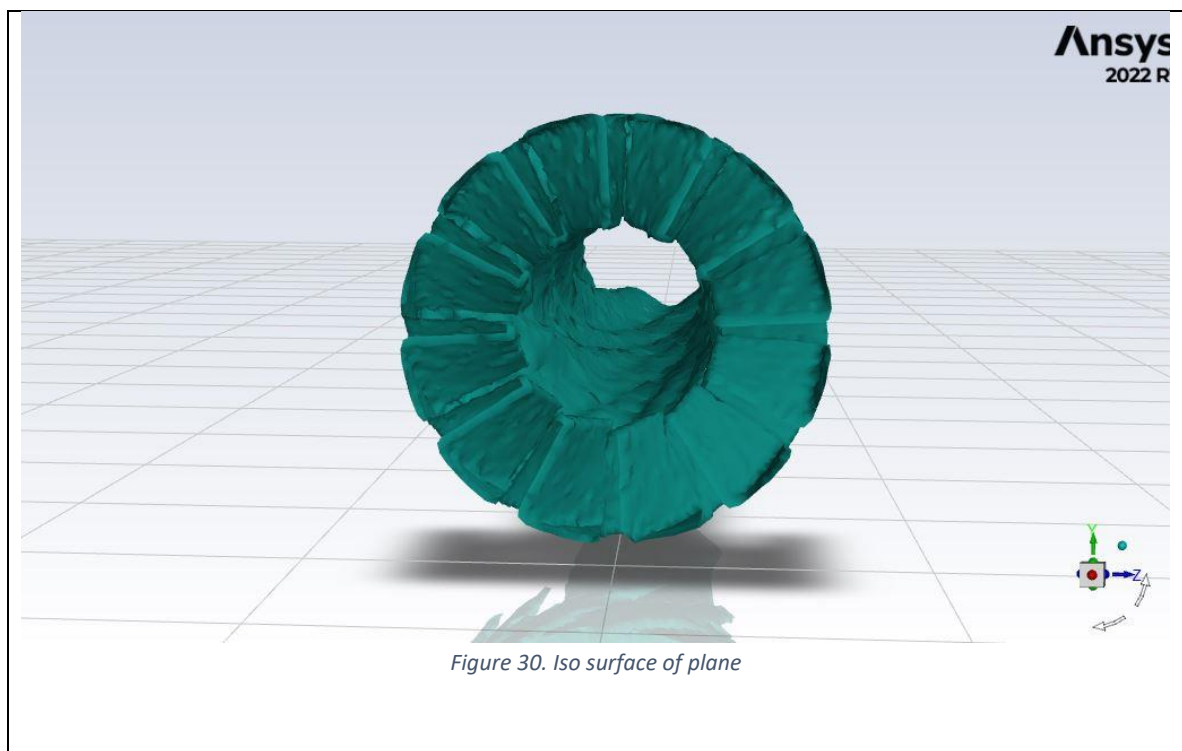
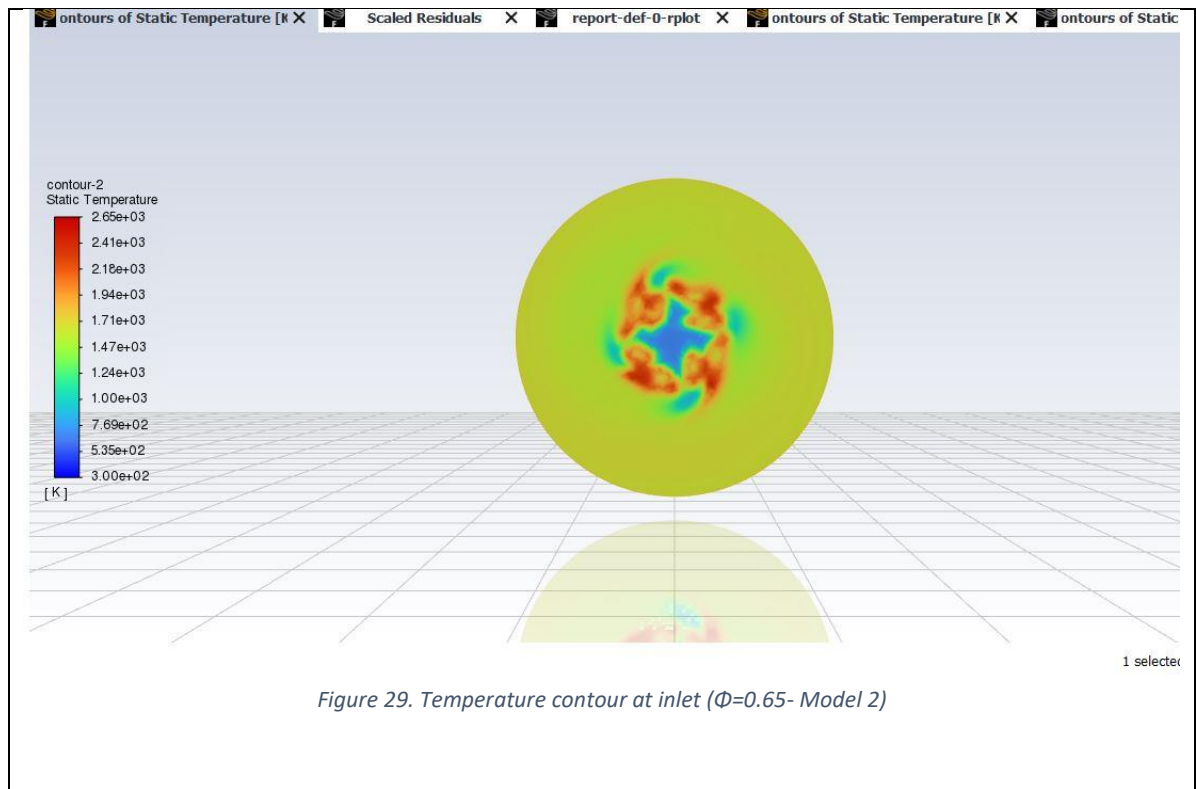
From Fig 26 and 27, as the swirler is introduced we can witness a slight increase in pressure drop. The swirler is meant to improve the mixing of air-fuel at the conjunction. The pressure drop is within range while improving the mixing characteristics.

As we can see from the figure that pressure loss across the combustion is very less compared to design 1. At combustor inlet we have inlet pressure of 15.3 atm and at the exit plane it reduces to 15.1 atm.

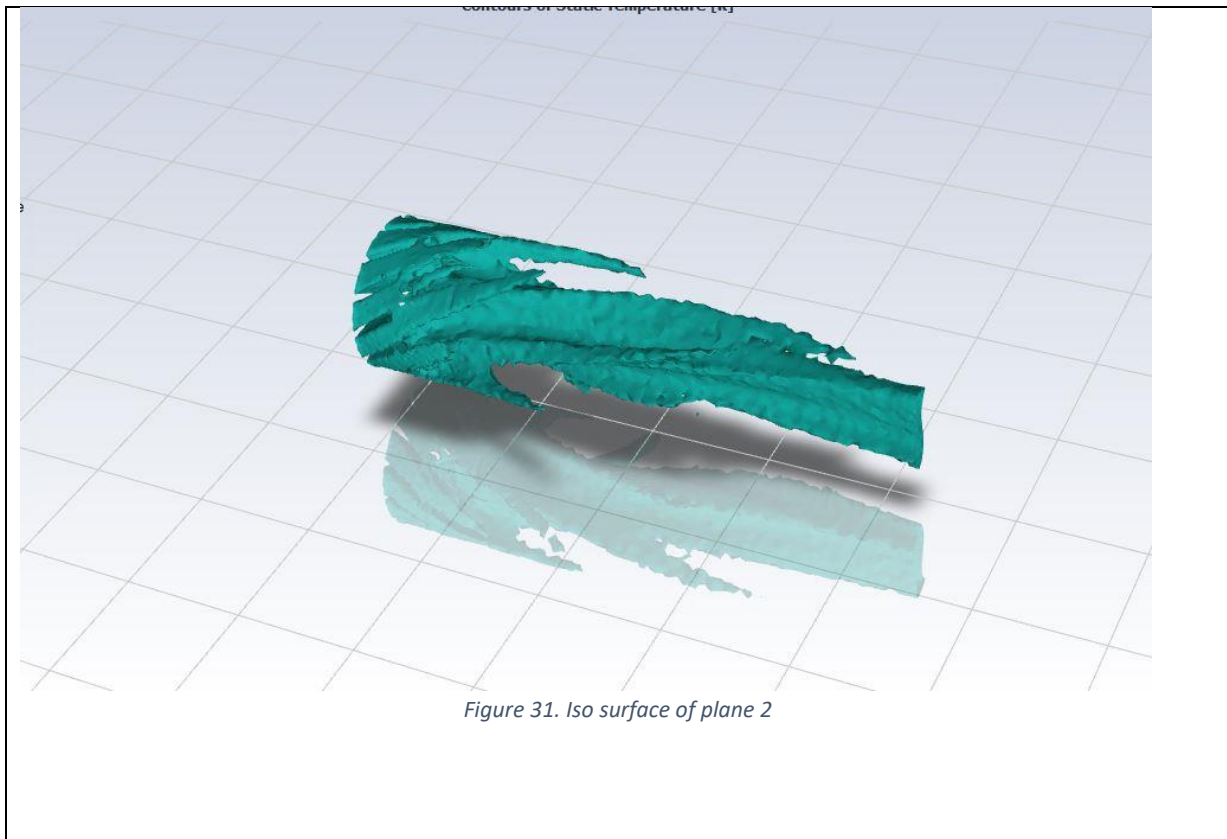


It is clear from figure that H₂ and Air is mixing at the end wall of the combustor. We have supplied our fuel on the periphery of the chamber which leads to create flame at that region only. Yellow and greenish region shows pre-combustion products and unburn O₂ which propagates forward and create flame region where temperature is around 2100K which is justifiable from the Cantera calculation we performed in hand calculation section.

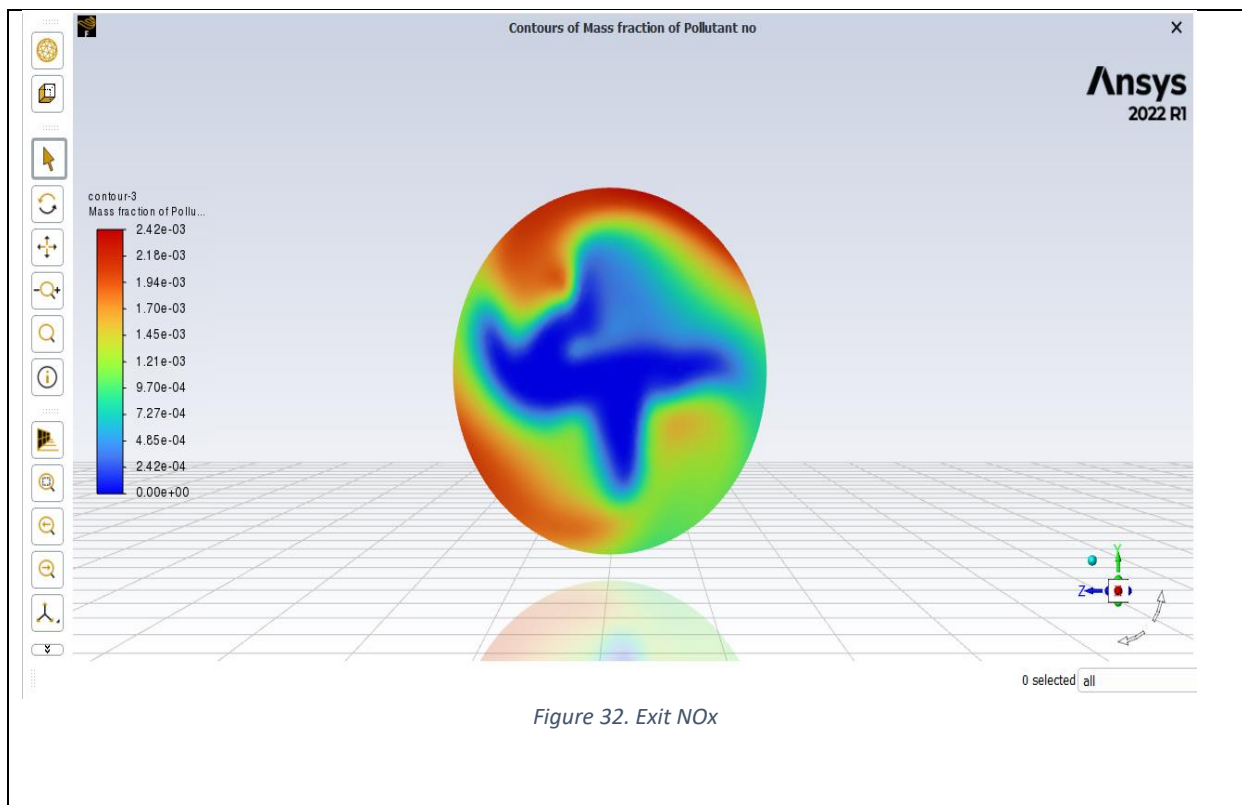
Red zone at the end of chamber shows unburn oxygen which is already present in the chamber and get heated up due to the flame temperature that has no concern with flame generation i.e., which does not show any flame region. It can be eliminated using wall cooling method by applying certain temperature. Also, computational software like Ansys Fluent needs basic understanding of fully developed flow and for that we have attach one dummy nozzle behind the combustion chamber.



Above fig shows iso surface of the flame. This iso surface has been created at the temperature of 1000K which clearly depicts that flame is getting formed across the periphery of the Nozzle. Which further propagate to the end of combustion chamber.



NOx contour at the exit of chamber



Calculated NOx at the exit of combustion chamber

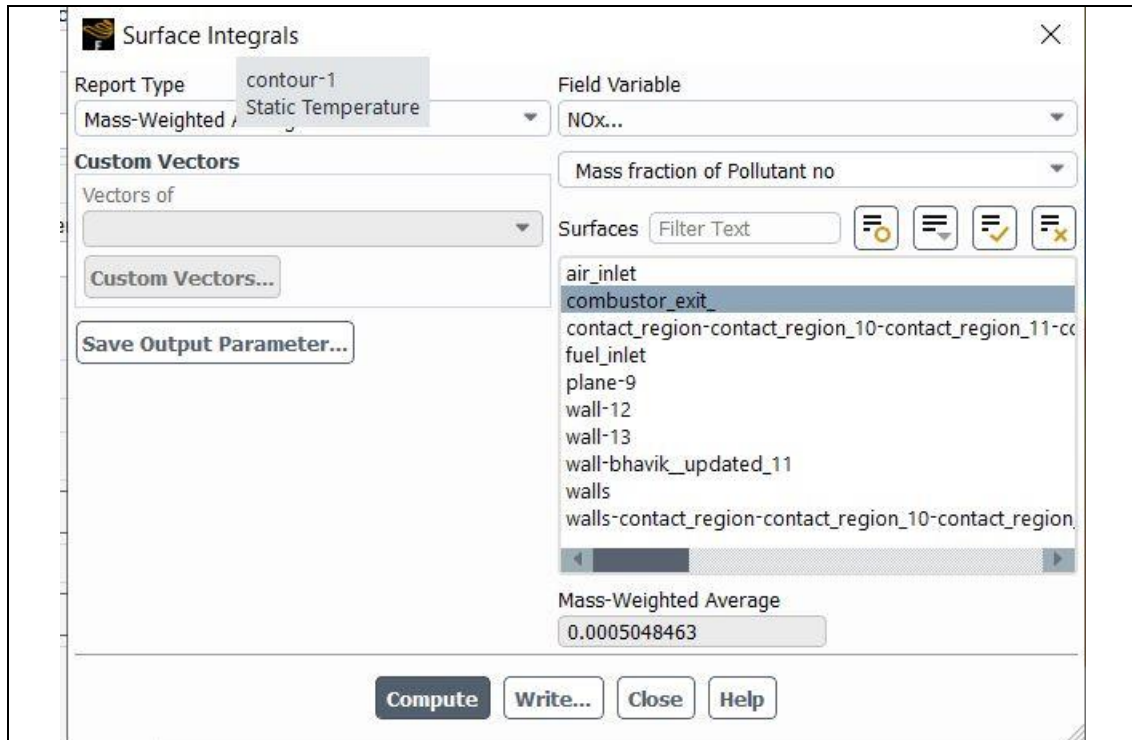


Figure 33. NOx at combustion chamber

Velocity Contour

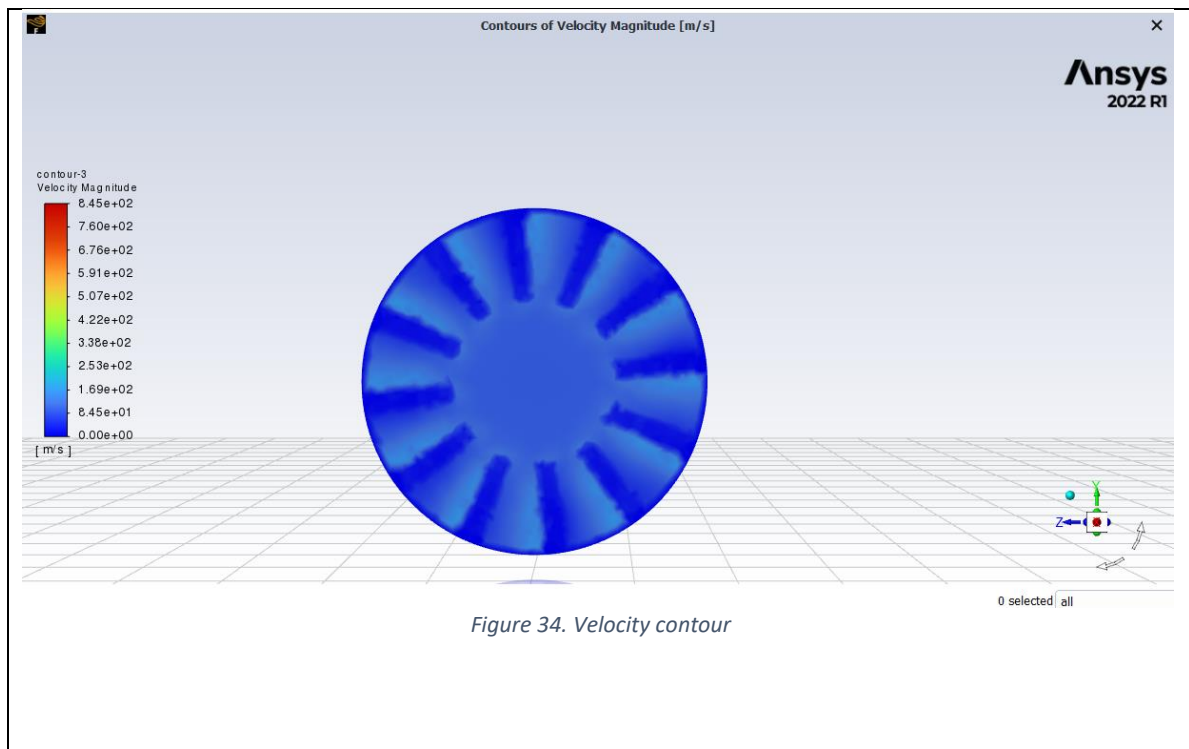
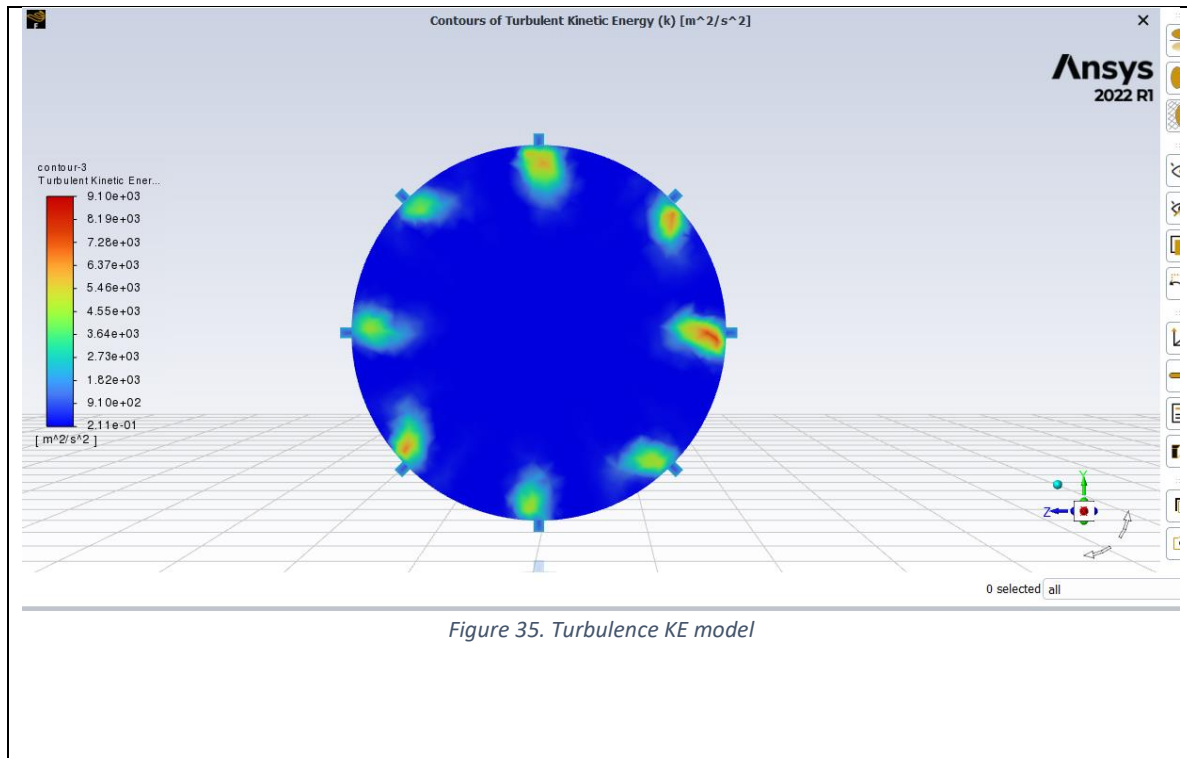


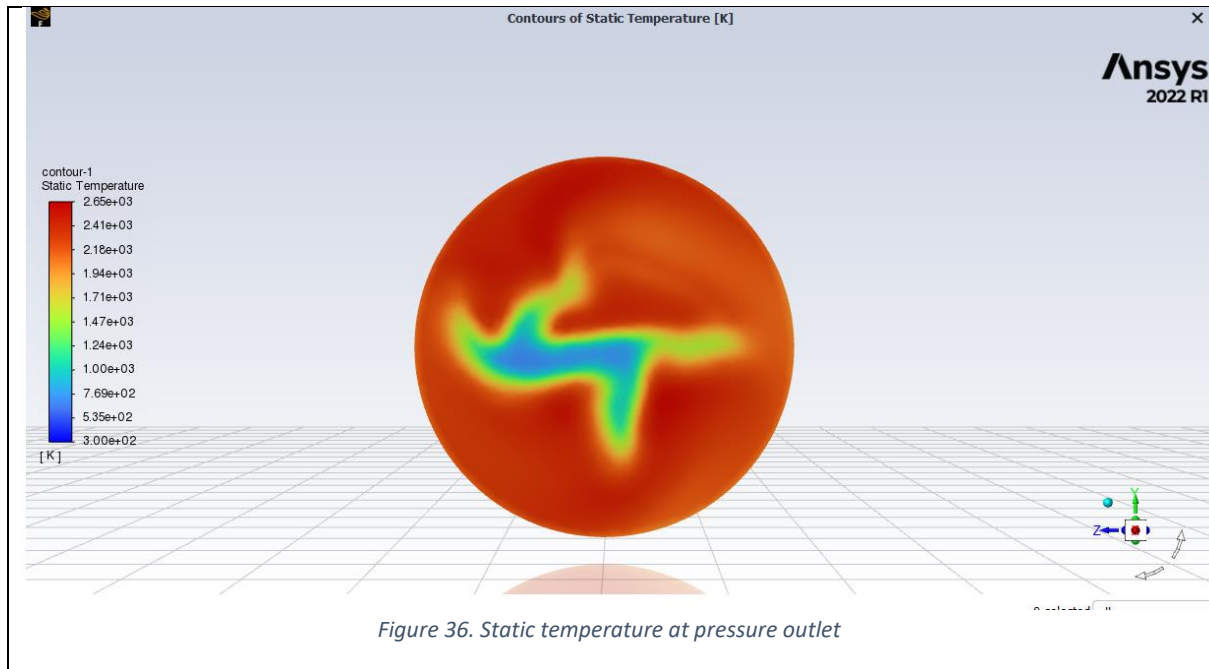
Figure 34. Velocity contour

Above fig shows velocity contours across the injector plane which shows raise in velocity due to swirl and recirculation of air.

Turbulence Kinetic energy model:



Above figure displays K-E turbulence model at fuel inlet plane which describes most of the mixing happens at fuel Injection points.



Results for Model-2 at an Equivalence ratio of 0.65

Pressure drops across the Injector	4%
Outlet Temperature	1700K (Considering flame only)
Nox	504PPM

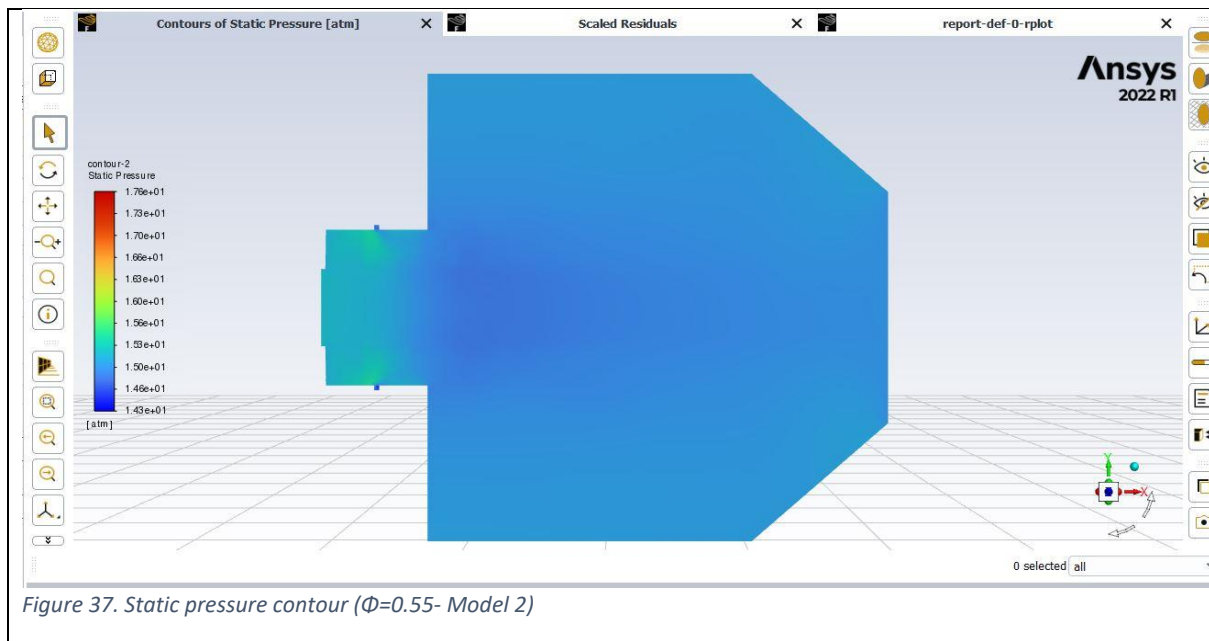
Table 12 Pressure drop at equivalence ratio 0.65

8.3 Results at design the equivalence ratio of 0.55

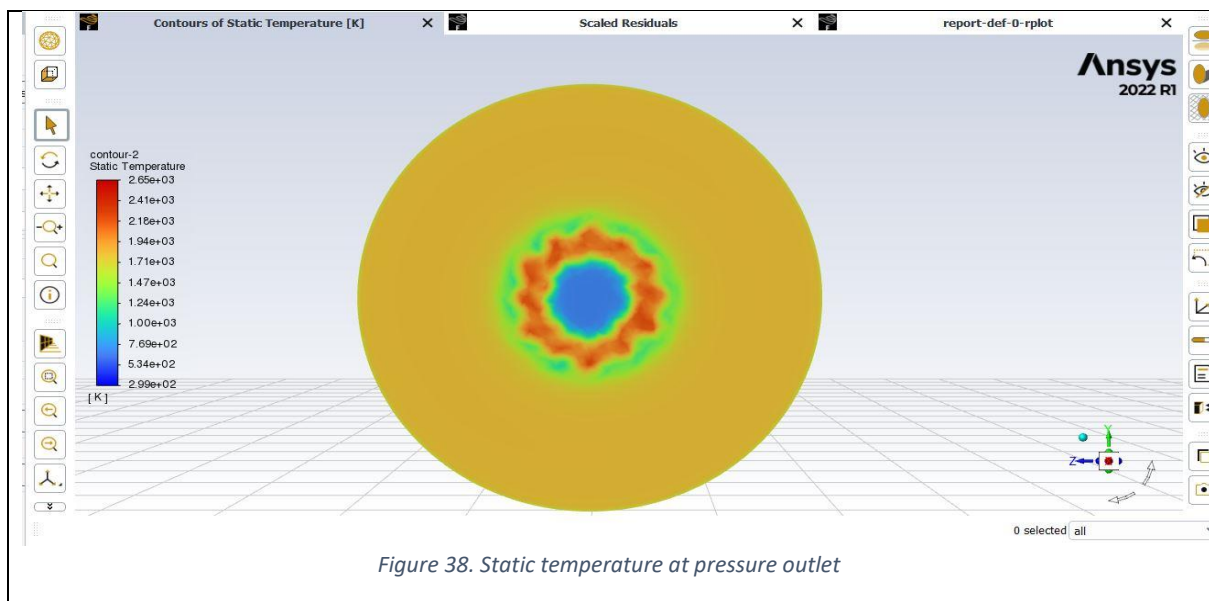
By reducing equivalence ratio, we are reducing fuel that is supplied for combustion. Which results into lower combustion temperature and as Ansys predict thermal NO_x based on zeldowich equation results into lower Nox at the exit of combustion chamber.

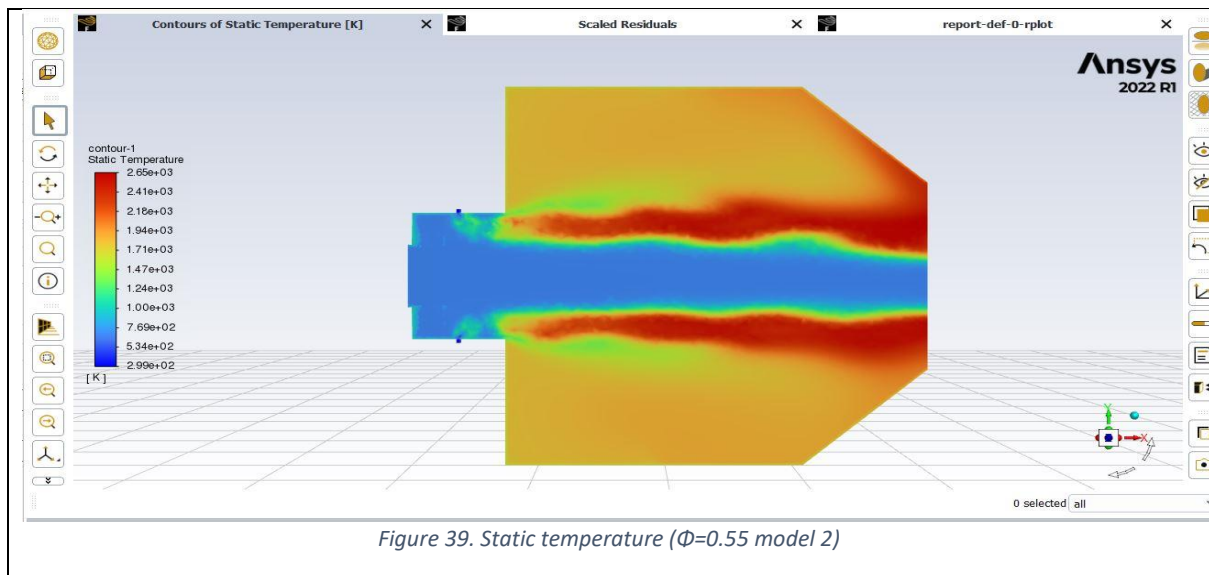
By changing equivalence ratio we are changing inlet velocity of fuel and air depending on the changes in mass flow rates.

Pressure Contour

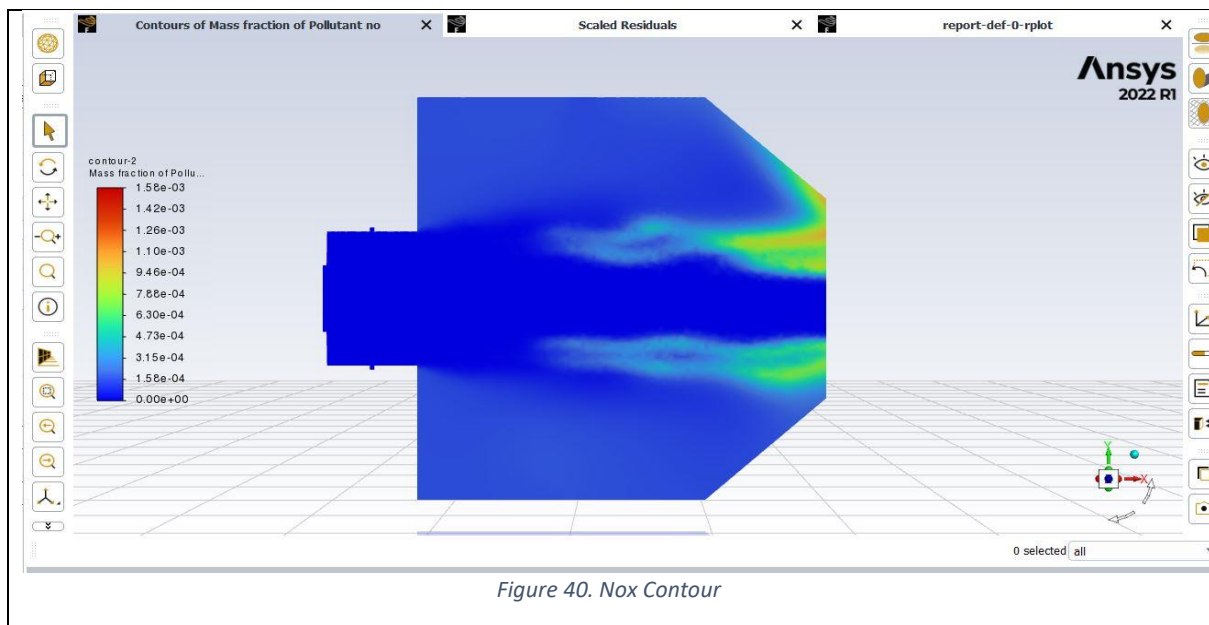


Temperature Contour at the exit of chamber

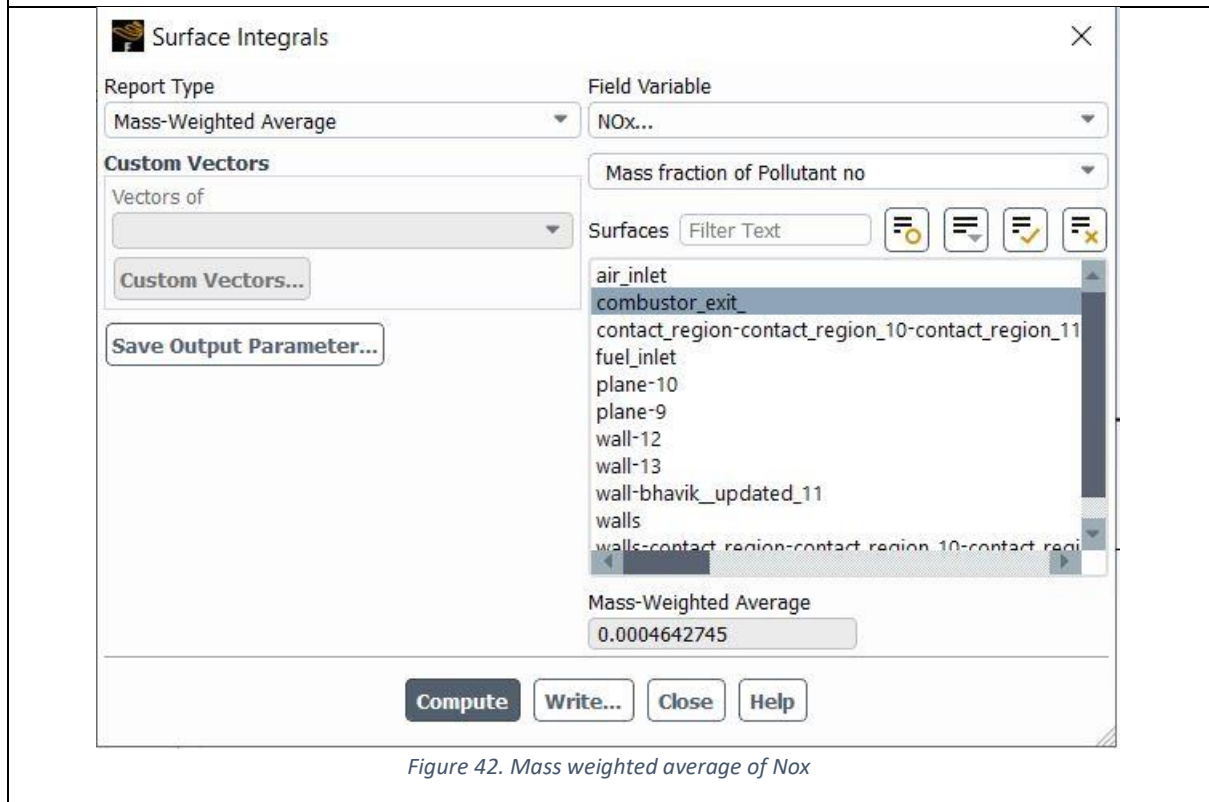
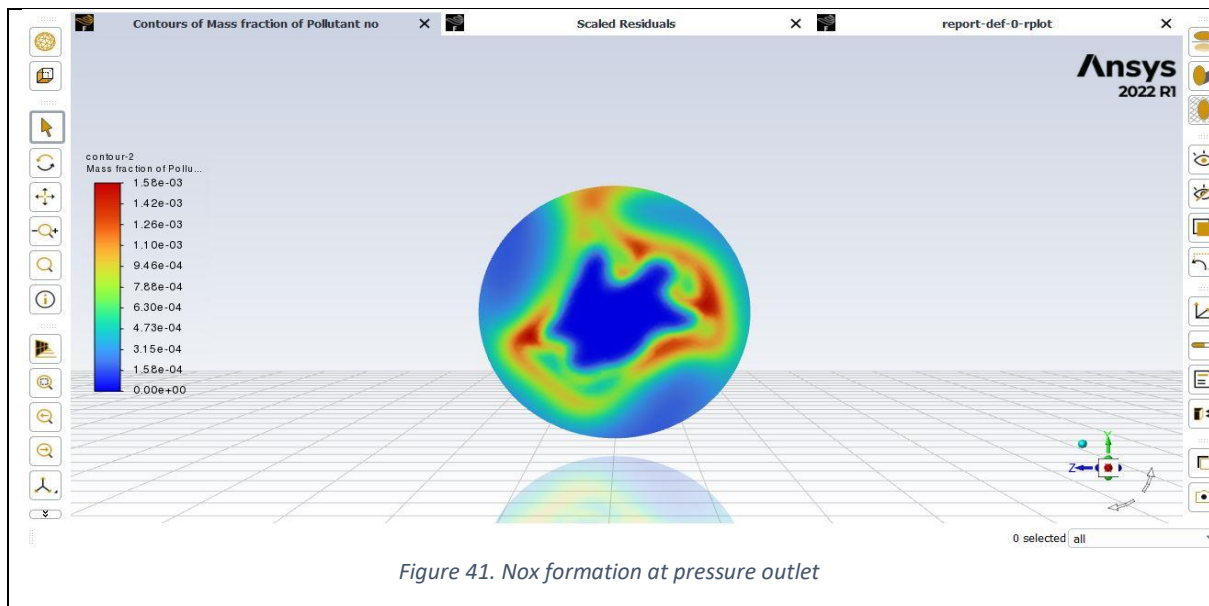




Nox Contour across chamber length



Thermal Nox at the exit of chamber



Results for Model-2 at an Equivalence ratio of 0.55

Pressure drop across the Injector	3.7%
Outlet Temperature	1640K (Considering flame only)
Nox	464 PPM

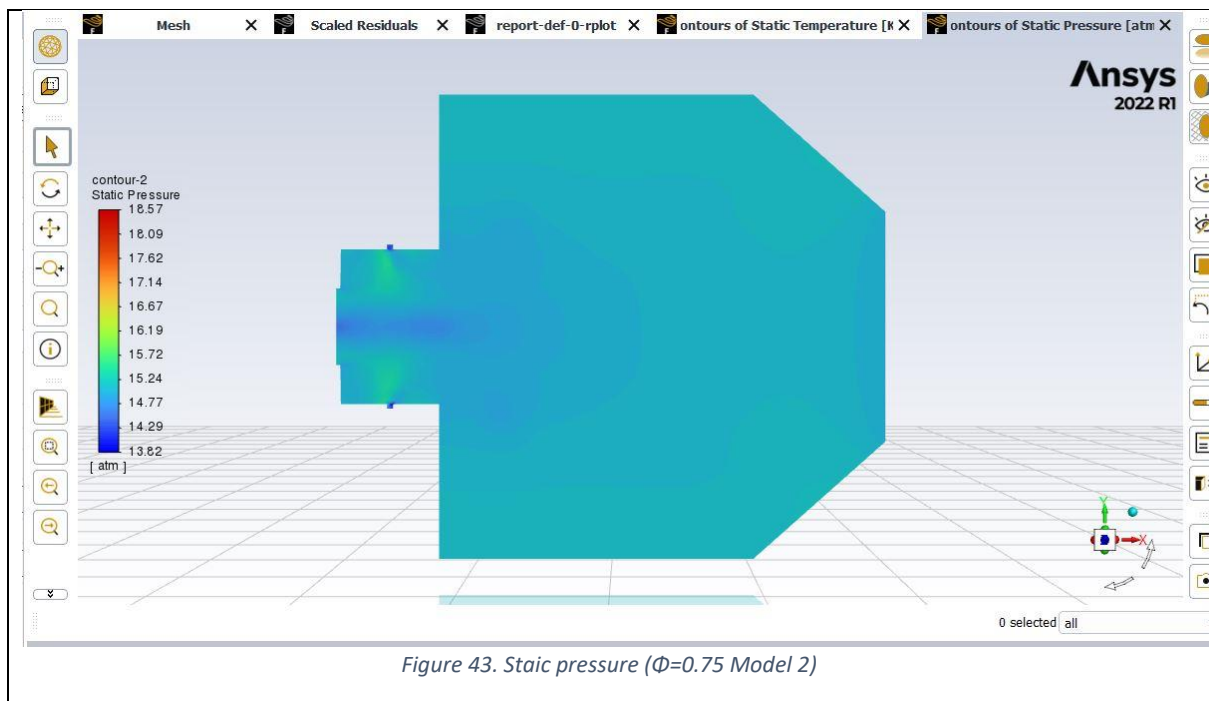
Table 13 Pressure drop at equivalence ratio 0.55

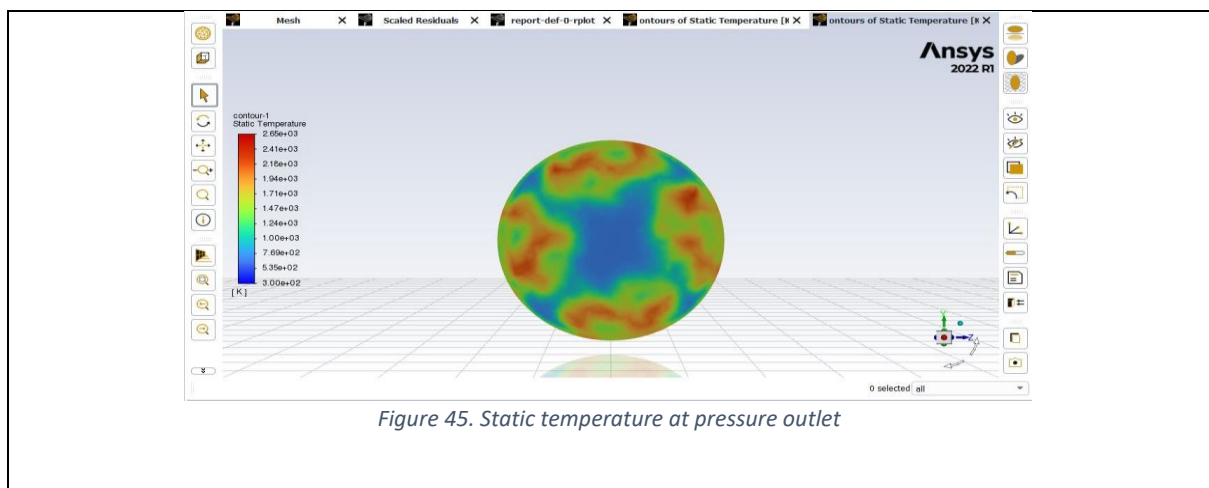
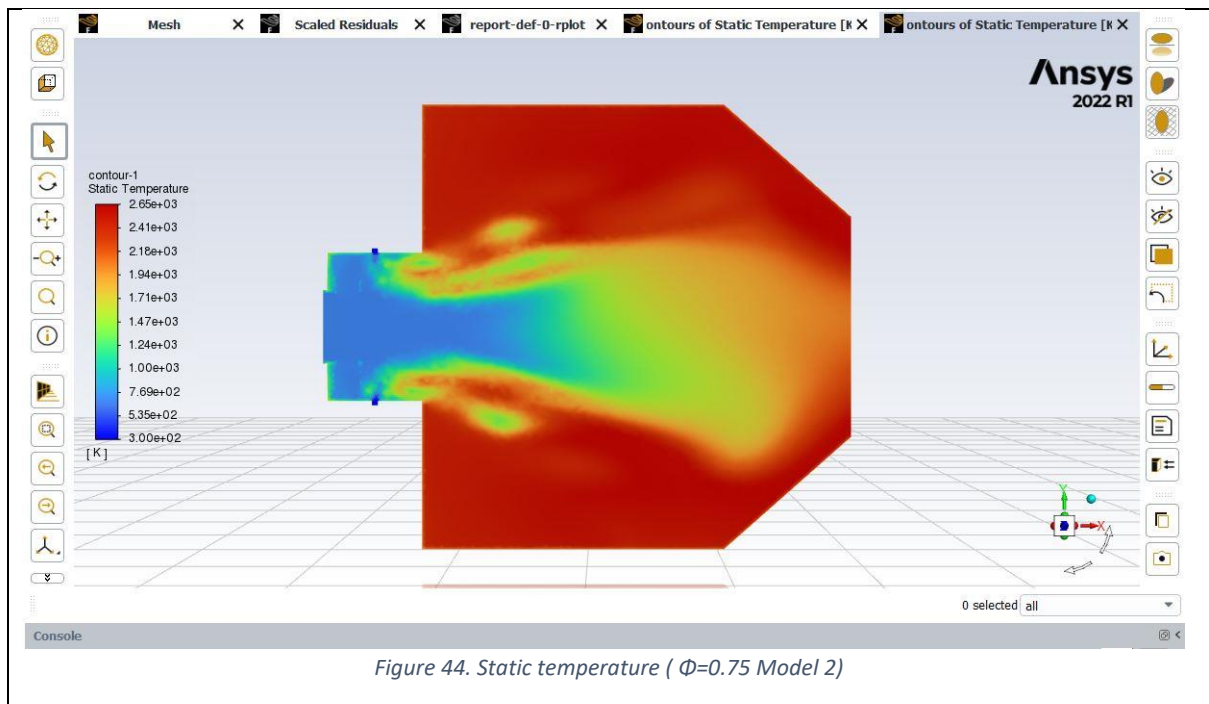
8.4 Results at design the equivalence ratio of 0.75

Pressure contour

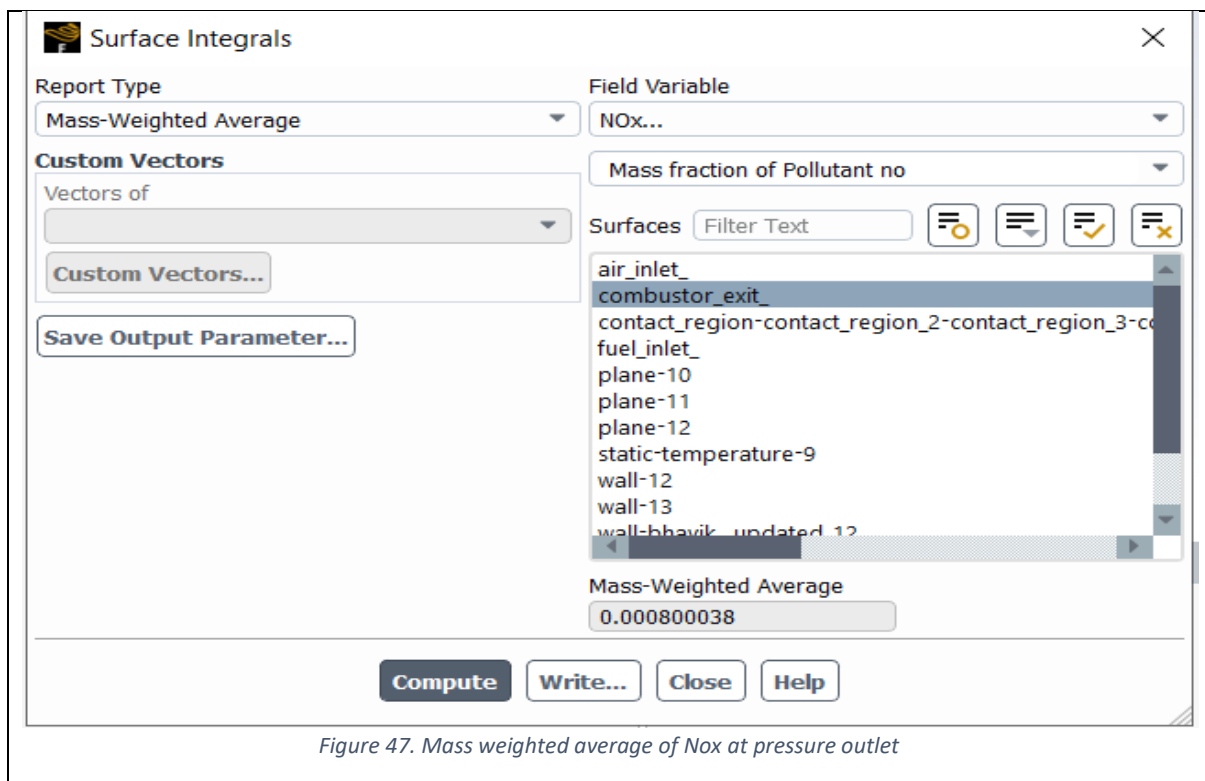
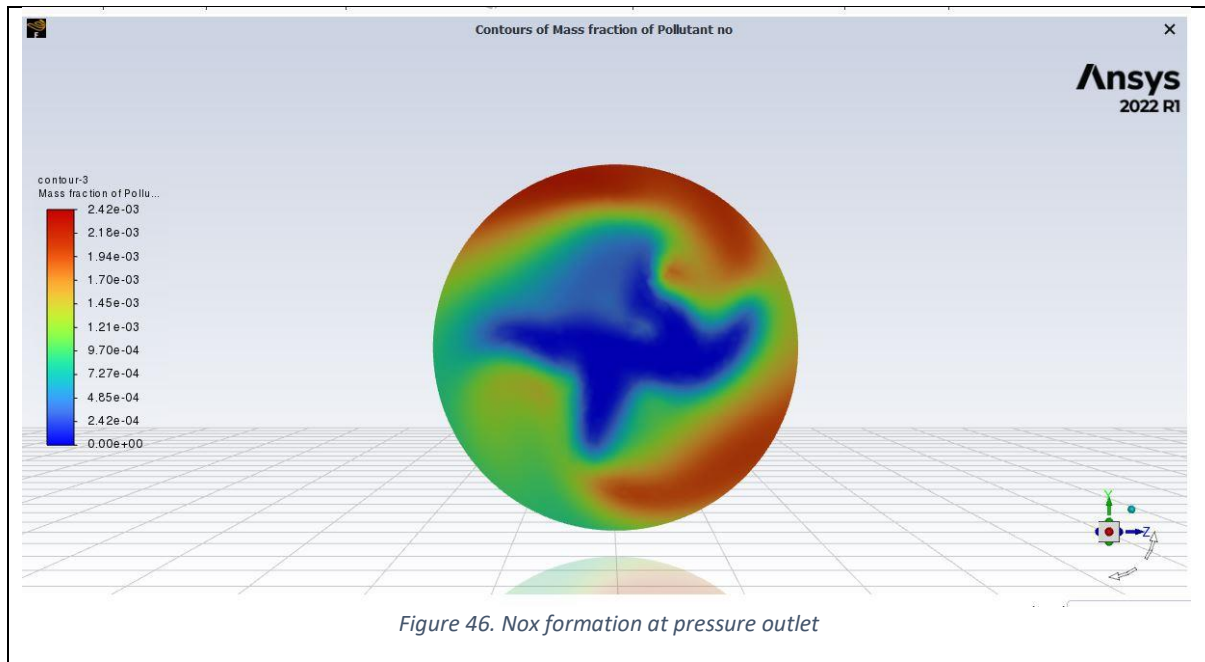
By Increasing equivalence ratio, we are increasing fuel that is supplied for combustion. Which results into higher combustion temperature and as Ansys predict thermal NO_x based on zeldowich equation results into higher NO_x at the exit of combustion chamber.

By changing equivalence ratio, we are changing inlet velocity of fuel and air depending on the changes in mass flow rates.





NOx Contour at the exit of combustor



Results for Model-2 at an Equivalence ratio of 0.75

Pressure drop across the Injector	4.1%
Outlet Temperature	1800 K (Considering flame only)
Nox	800 PPM

Table 14 Pressure drop at equivalence ratio 0

9. Conclusion:

This report covered the design of an injector with hydrogen as the primary fuel source. The reason of using hydrogen was to reduce the NOx emissions. Rigorous design changes were conducted in order to stick with the solution output i.e., reduced NOx. All the presented designs were simulated through various equivalence ratios supported by hand calculations. The best result that we calculated was on the second design with equivalence ratio of 0.55 where we marked NOx emission of 464PPM and 3.7% of Pressure loss across the injector.

We used the comparison method where we take reference from our old design considerations and try to remodel it for better results. Initially, in the first Model where we got NOx emission of 861PPM and 5% pressure loss, we injected fuel in direct perpendicular direction of the airflow which was in axial direction. There we noticed the incomplete combustion as the mixing of air and fuel was up to mark. By considering that factor, we introduced swirl in our design. Due to which we observed better mixing of the fuel with air and thus reduced NOx emissions.

Although the results which we got are far different from the industrial NOx standard. There are many reasons in support of this far difference such as due to limitations in the computational power we were not able to generate the targeted quality of mesh. Apart from that flow modelling could have been improvised using many methods. As per our experience we tried another design modification in which fuel inlet ports are located inside of the swirler hub which gives an efficient recirculation of air, and which mix with fuel immediately. Although the fabrication of such design is quite challenging as it involves peripheral drilling on the hub surface.

Also, we can try introducing baffle plates which create recirculation paths for incoming air. But in that were we were restricted by the flow conditions which we can use as we were getting flashbacks for the selected range of equivalence ratios which we used.

10. References:

- [1] B. Khandelwal, Y. Li, P. Murthy, V. Sethi, and R. Singh, "Implication of Different Fuel Injector Configurations for Hydrogen Fuelled Micromix Combustors," pp. 1–6, 2011.
- [2] X. Sun, P. Agarwal, F. Carbonara, D. Abbott, P. Gauthier, and B. Sethi, "Numerical Investigation into the Impact of Injector Geometrical Design Parameters on Hydrogen Micromix Combustion Characteristics," pp. 1–11, 2020.
- [3] O. Reddy and K. M. Pandey, "Hydrogen fueled scramjet combustor with a wavy-wall double strut fuel injector," *Fuel*, vol. 304, no. May, p. 121425, 2021, doi: 10.1016/j.fuel.2021.121425.
- [4] Ali Cemal Benim, Khawar Syed, Flashback Mechanisms in Lean Premixed Gas Turbine Combustion, (2015)
- [5] <https://www.energy.gov/eere/fuelcells/liquid-hydrogen-delivery>
- [6] <https://doi.org/10.1016/j.pecs.2021.100907>
- [7] <https://alternative-fuels-observatory.ec.europa.eu/transport-mode/aviation/alternative-fuels-for-aviation>
- [8] <chrome-extension://efaidnbmnnnibpcajpcglclefindmkaj/https://alfaproject.ir/wp-content/uploads/2020/06/part14.pdf>
- [9] <https://www.afs.enea.it/project/neptunius/docs/fluent/html/th/node142.htm>
- [10] <https://www.afs.enea.it/project/neptunius/docs/fluent/html/th/node112.htm>
- (I) https://www.researchgate.net/figure/Cutaway-view-of-typical-industrial-gas-turbine-engine-obtained-from-Britannica_fig6_288707880