



**Combustion of Premixed Propane and Air CFD Analysis
MECH 6191**

Final Project

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INTRODUCTION

As the complexity of jet engine increases, costly experimental procedures are required to test its performance parameters. This has been the motivation for using flow simulations, or Computational Fluid Dynamics (CFD) for predicting fluid flow, heat transfer, mass transfer, chemical reactions, and related phenomena by solving numerical methods [1]. CFD has also been a great tool to gain insight and understanding in the predictions of flow fields, temperature field, species concentrations, and particulates and pollutants. Focusing on the combustion process, literature shows that this complex phenomenon is still an area of great research [2]. The complexity comes from the effects of turbulence on the reacting fluid. Reactions and turbulence affect each other through flow acceleration and modified kinematic viscosity. The modified turbulence affects the flame structure and enhances the mixing and chemical reactions [2]. This project focuses on the use of CFD to obtain numerical results for the premixed stoichiometric and lean combustion reaction of Propane and air. The premixed flame assumes that the fuel and oxidizer are already mixed at the molecular level prior to ignition. The software ANSYS and its postprocessing tools are used to run the CFD analysis. The combustion system is formed by introducing combustion chamber geometry and creating a mesh finely-tuned for the most accurate solution generation. The main focus of the post-processing analysis will be on the mass and molar mass fractions of the product species related to the reaction. Furthermore, the adiabatic flame temperature is also studied and calculated. Finally, the solutions of the model products and temperatures will be compared to analytical calculations.

1.1. Background

Computational fluid dynamics (CFD) is a branch of fluid mechanics that uses different numerical analysis methods to solve and analyze flow phenomenon. The emergence of computational fluid dynamics has promoted the development of fluid machinery research which was originally developed from the pioneering accomplishments of enthusiasts such as Richardson (1910) and Courant, Friedrichs, and Lewy (1928). With the rapid development of computer technology, CFD technology has developed rapidly and has gradually become an important means of product development along with experimental fluid mechanics.

The Finite Volume Method (FVM) is one of the widely used numerical techniques in solving the partial differential equations in the conservation laws of fluid dynamics. This method transforms differential volume into the discrete algebraic equation on finite volume. Then, the algebraic equations are solved to calculate the dependent variables of each element to represent the physical process. ANSYS Fluent is a commercial CFD code based on the finite volume method, which contains many turbulence models and can simulate the steady or unsteady state of viscous or non-viscous fluids.

1.2. Theory

The objective of the project is to model viscous flow in a premixed flame combustor dealing with propane by solving the Navier-Stokes equations with appropriate boundary conditions using the Ansys Fluent CFD software which uses the Finite Volume Method. The basic idea of the finite volume method is to divide the computational region into a series of non-repetitive control volumes and make each grid point surrounded by a control volume. By integrating the differential equation to be solved with each control volume, a set of discrete equations can be obtained. The unknown is the value of the dependent variable at the grid point. In order to obtain the integral of the control volume, it is necessary to assume that the distribution profile of the hypothetical value is divided into segments. From the point of view of the selection method of the integral region, the finite volume method belongs to the sub-region method of weighted residuals and from the point of view of the approximation method of the unknown solution, the finite volume method belongs to the discrete method of local approximation. In short, the sub-region method belongs to the basic method of finite volume generation.

1.3. Equations

1.3.1. The Mass Conservation Equation

The equation for conservation of mass, or continuity equation, can be written as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m \quad (1.1)$$

The source S_m is the mass added to the continuous phase from the dispersed second phase (for example, due to vaporization of liquid droplets) and any user-defined sources.

For 2-D axisymmetric geometries, the continuity equation is given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial r}(\rho v_r) + \frac{\rho v_r}{r} = S_m \quad (1.2)$$

Where x is the axial coordinate, r is the radial coordinate, v_x is the axial velocity, and v_r is the radial velocity.

1.3.2. Momentum Conservation Equation

Conservation of momentum in an inertial (non-accelerating) reference frame is given by

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\vec{\tau}) + \rho \vec{g} + \vec{F} \quad (1.3)$$

where p is the static pressure, $\vec{\tau}$ is the stress tensor (described below), and $\rho \vec{g}$ and \vec{F} are the gravitational body force and external body forces (for example, that arise from interaction with the dispersed phase), respectively. \vec{F} also contains other model-dependent source terms such as porous-media and user-defined sources.

The stress tensor $\vec{\tau}$ is given by

$$\vec{\tau} = \mu \left[\left(\nabla \vec{v} + \nabla \vec{v}^T \right) - \frac{2}{3} \nabla \cdot \vec{v} I \right] \quad (1.4)$$

where μ is the molecular viscosity, I is the unit tensor, and the second term on the right-hand side is the effect of volume dilation.

For 2-D axisymmetric geometries, the axial and radial momentum conservation equations are given by

$$\begin{aligned}
\frac{\partial}{\partial t}(\rho v_x) + \frac{1}{r} \frac{\partial}{\partial x}(r \rho v_x v_x) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v_r v_x) = & -\frac{\partial p}{\partial x} \\
& + \frac{1}{r} \frac{\partial}{\partial x} \left[r \mu \left(2 \frac{\partial v_x}{\partial x} - \frac{2}{3} (\nabla \cdot \vec{v}) \right) \right] \\
& + \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(\frac{\partial v_x}{\partial r} + \frac{\partial v_r}{\partial x} \right) \right] + F_x
\end{aligned} \tag{1.5}$$

and

$$\begin{aligned}
\frac{\partial}{\partial t}(\rho v_r) + \frac{1}{r} \frac{\partial}{\partial x}(r \rho v_x v_r) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v_r v_r) = & -\frac{\partial p}{\partial r} \\
& + \frac{1}{r} \frac{\partial}{\partial x} \left[r \mu \left(\frac{\partial v_r}{\partial x} + \frac{\partial v_x}{\partial r} \right) \right] \\
& + \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(2 \frac{\partial v_r}{\partial r} - \frac{2}{3} (\nabla \cdot \vec{v}) \right) \right] \\
& - 2\mu \frac{v_r}{r^2} + \frac{2}{3} \frac{\mu}{r} (\nabla \cdot \vec{v}) + \rho \frac{v_z^2}{r} + F_r
\end{aligned} \tag{1.6}$$

where

$$\nabla \cdot \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} + \frac{v_r}{r} \tag{1.7}$$

and v_z is the swirl velocity.

1.4. Terminology

Φ - equivalence ratio

$\Delta H = 0$ – Change in Enthalpy

T_f - Adiabatic Flame Temperature

n_T – Total Number of Moles

2. PROJECT DESCRIPTION

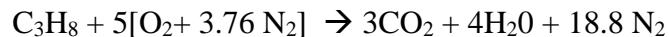
First, the analytical calculations of the overall chemical equations for the complete combustion of propane and air are performed with the assumption of no product dissociation. The product mole ratios are taken from the stoichiometric and lean ($\phi = 0.75$) chemical equations for the two inlet mixture conditions of the simulations. It is assumed that Propane (C_3H_8) gas, supplied at 1atm and 298K, is burned adiabatically in a steady-flow burner with air supplied at the same pressure and temperature.

For the stoichiometric and lean ($\phi = 0.75$) chemical reactions, the flame temperature, mole fraction of products, mass fraction of products are calculated analytically and compared with numerical results from the simulation.

3. RESULTS

3.1. Analytical Results

3.1.1. Stoichiometric condition for Propane



Complete and Stoichiometric Combustion: Full utilization of fuel and air in the generation of combustion products was assumed along with no product dissociation.

a) Flame Temperature

$$\Delta H = 0$$

$$\{3\Delta h_{CO_2}^0 + 4\Delta h_{H_2O}^0 - \Delta h_{C_3H_8}^0\} + 3\{h_{CO_2}(T_f) - h_{CO_2}(298)\} + 1\{h_{H_2O}(T_f) - h_{H_2O}(298)\} + 18.8\{h_{N_2}(T_f) - h_{N_2}(298)\} = 0$$

Let $T_f = 2400$ K,

$$\{3(-94.054) + 4(-57.798) - (-25.02)\} + 3(27.672) + 4(22.405) + 18.8(16.883) = 0$$

- 488.33 + 490.04 = 0 Too Hot!

Let $T_f = 2200$ K,

$$\{3(-94.054) + 4(-57.798) - (-25.02)\} + 3(24.752) + 4(19.874) + 18.8(15.144) = 0$$

$$-488.33 + 438.46 = 0 \quad \text{Too Cold!}$$

Therefore, by interpolation,

$$\frac{488.33 - 438.46}{490.04 - 438.46} = \frac{x - 2200}{2400 - 2200}$$

$$T_f = 2393.37 \text{ K}$$

b) Mole fractions of products at the combustor exit plane

$$\text{Total number of moles in the products, } n_T = 3 + 4 + 18.8 = 25.8$$

$$\text{Mole Fraction of CO}_2 = 3 / 25.8 = 0.116$$

$$\text{Mole Fraction of H}_2\text{O} = 4 / 25.8 = 0.155$$

$$\text{Mole Fraction of N}_2 = 18.8 / 25.8 = 0.728$$

c) Mass fractions of products at the combustor exit plane

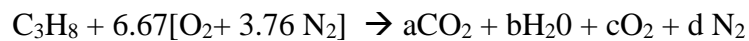
$$\begin{aligned} \text{Total Mass of the products} &= 3\{12 + 2(16)\} + 4\{2(1) + 16\} + 18.8\{2(14)\} \\ &= 730.4 \end{aligned}$$

$$\begin{aligned} \text{Mass Fraction of CO}_2 &= \frac{3\{12 + 2(16)\}}{730.4} \\ &= 0.1807 \end{aligned}$$

$$\begin{aligned} \text{Mass Fraction of H}_2\text{O} &= \frac{4\{2(1) + 16\}}{730.4} \\ &= 0.0986 \end{aligned}$$

$$\begin{aligned} \text{Mass Fraction of N}_2 &= \frac{18.8\{2(14)\}}{730.4} \\ &= 0.720 \end{aligned}$$

3.1.2. Lean Condition for Propane ($\phi = 0.75$)



Element Balance:

$$\text{C: } 3 = a$$

$$\text{H: } 8 = 2b \rightarrow b=4$$

$$\text{O: } 13.34 = 2a + b + 2c \rightarrow c = 1.67$$

$$\text{N: } 50.16 = 2d \rightarrow d = 25.08$$



a) Flame Temperature

$$\Delta H = 0$$

$$\{3\Delta h_{\text{CO}_2}^0 + 4\Delta h_{\text{H}_2\text{O}}^0 - \Delta h_{\text{C}_3\text{H}_8}^0\} + 3\{h_{\text{CO}_2}(T_f) - h_{\text{CO}_2}(298)\} + 4\{h_{\text{H}_2\text{O}}(T_f) - h_{\text{H}_2\text{O}}(298)\} + 1.67\{h_{\text{O}_2}(T_f) - h_{\text{O}_2}(298)\} + 25.08\{h_{\text{N}_2}(T_f) - h_{\text{N}_2}(298)\} = 0$$

$$\text{Let } T_f = 2400 \text{ K}$$

$$\{3(-94.054) + 4(-57.798) - (-25.02)\} + 3(27.672) + 4(22.405) + 1.67(17.795) + 25.08(16.883) = 0$$
$$-488.33 + 625.77 = 0 \quad \text{Too Hot!}$$

$$\text{Let } T_f = 2000 \text{ K}$$

$$\{3(-94.054) + 4(-57.798) - (-25.02)\} + 3(21.854) + 4(17.397) + 1.67(14.143) + 25.08(13.417) = 0$$
$$-488.33 + 495.26 = 0 \quad \text{Hot!}$$

$$\text{Let } T_f = 1900 \text{ K}$$

$$\{3(-94.054) + 4(-57.798) - (-25.02)\} + 3(20.416) + 4(16.182) + 1.67(13.244) + 25.08(12.559) = 0$$
$$-488.33 + 463.07 = 0 \quad \text{Cold!}$$

Therefore, by interpolation,

$$\frac{488.33 - 463.07}{495.26 - 463.07} = \frac{x - 1900}{2000 - 1900}$$
$$T_f = 1981.58 \text{ K}$$

b) Mole fractions of products at the combustor exit plane

Total number of moles in the products, $n_T = 3 + 4 + 1.67 + 25.08 = 33.75$

Mole Fraction of $\text{CO}_2 = 3 / 33.75 = 0.0889$

Mole Fraction of $\text{H}_2\text{O} = 4 / 33.75 = 0.1185$

Mole Fraction of $\text{O}_2 = 1.67 / 33.75 = 0.0495$

Mole Fraction of $\text{N}_2 = 25.08 / 33.75 = 0.743$

c) Mass fractions of products at the combustor exit plane

Total Mass of the products = $3\{12 + 2(16)\} + 4\{2(1) + 16\} + 1.67\{2(16)\} + 25.08\{2(14)\}$
 $= 959.68$

Mass Fraction of $\text{CO}_2 = \frac{3\{12 + 2(16)\}}{959.68}$
 $= 0.137$

Mass Fraction of $\text{H}_2\text{O} = \frac{4\{2(1) + 16\}}{959.68}$
 $= 0.075$

Mass Fraction of $\text{O}_2 = \frac{1.67\{2(16)\}}{959.68}$
 $= 0.0557$

Mass Fraction of $\text{N}_2 = \frac{25.08\{2(14)\}}{959.68}$
 $= 0.731$

3.2. Numerical Results

In this section, CFD results are demonstrated for the Adiabatic Flame Temperature, Mole fraction distribution and Mass fraction distribution of propane combustion. The simulation has

been first performed for the stoichiometric reaction and then followed by a lean ($\phi = 0.75$) reaction. Both of the models are run for at least 1000 iterations in the CFD ANSYS simulation.

3.2.1. Set up:

- The simulation is set up to be “steady”
- The effects of turbulence are modelled by increasing the viscous effect and its kinetic energy (K). Also, viscosity is increased to simulate a slow reaction
- Volumetric combustion is turned on
- Eddy dissipation and K-omega are set for the chemistry turbulent interaction
- The incompressible ideal gas relationship is used
- The “simple” scheme is used for pressure-velocity couple. This decouples the relationship by solving for the velocity at constant pressure and update the velocity. Then a new pressure is used to update the next velocity and so on.
- The “second-order derivative” is used for better accuracy of calculation
- In this case, we have one inlet mixture boundary condition for the premixed gas of propane and air.
- The mole fractions are changed accordingly for the product composition of stoichiometric and lean reaction.

Mole Fraction and mass fraction calculations from CFD for Stoichiometric and lean reaction

Mole Fraction and mass fraction calculations from CFD is obtained from function calculator from CFD Post software. Example result for H₂O mole fraction is depicted below (the same procedure has been done for all other products and included in the table).

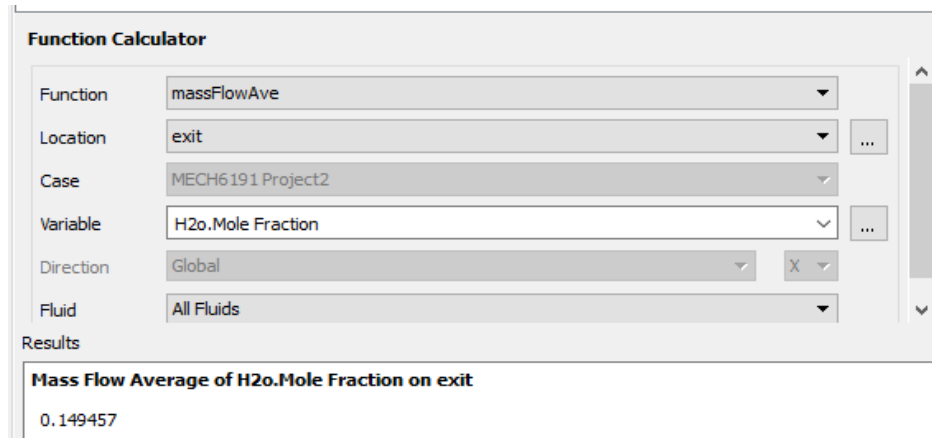


Figure 1. Function Calculator for mole fraction at exit plane

3.2.2. Stoichiometric Condition for Propane

a) Adiabatic Flame Temperature

Figure 2. demonstrates the temperature distribution along the can chamber. It starts with the set gas mixture temperature of 298 K as seen in the blue region. The colour change demonstrates the increase of temperature as gasses are heated to reach ignition temperature. The red area depicts the final flame temperature of 2376 K at the stoichiometric condition.

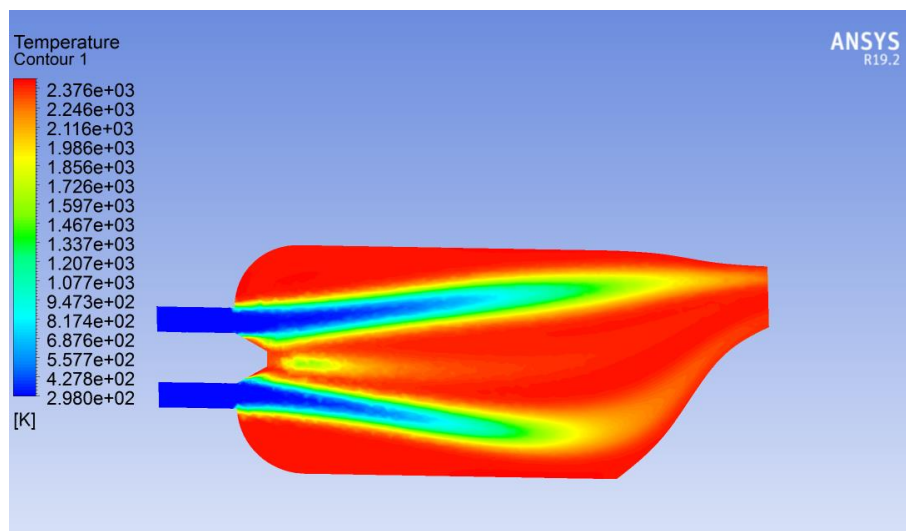


Figure 2. Stoichiometric Adiabatic Flame Temperature

a) Mole fractions of products at the combustor exit plane

| H ₂ O (CFD) | CO ₂ (CFD) | N ₂ (CFD) |
|------------------------|-----------------------|----------------------|
| 0.149 | 0.112 | 0.729 |

Table 1. Mole Fraction of Products at Exit Plane (Stoichiometric Reaction)

b) Mass fractions of products at the combustor exit plane

| H ₂ O(CFD) | CO ₂ (CFD) | N ₂ (CFD) |
|-----------------------|-----------------------|----------------------|
| 0.095 | 0.174 | 0.720 |

Table 2. Mass Fraction of Products at Exit Plane (Stoichiometric Reaction)

The mass fraction distributions of each species are obtained from the CFD analysis along the cross-section of the can chamber for the stoichiometric reaction.

Figure 3. demonstrates the H₂O mass fraction distribution along the can chamber. The blue region shows zero H₂O composition at the inlet and as the reaction proceeds, H₂O is formed and its composition is increased. After complete combustion, the final mass fraction composition of H₂O is shown by the orange region to be of about 0.095.

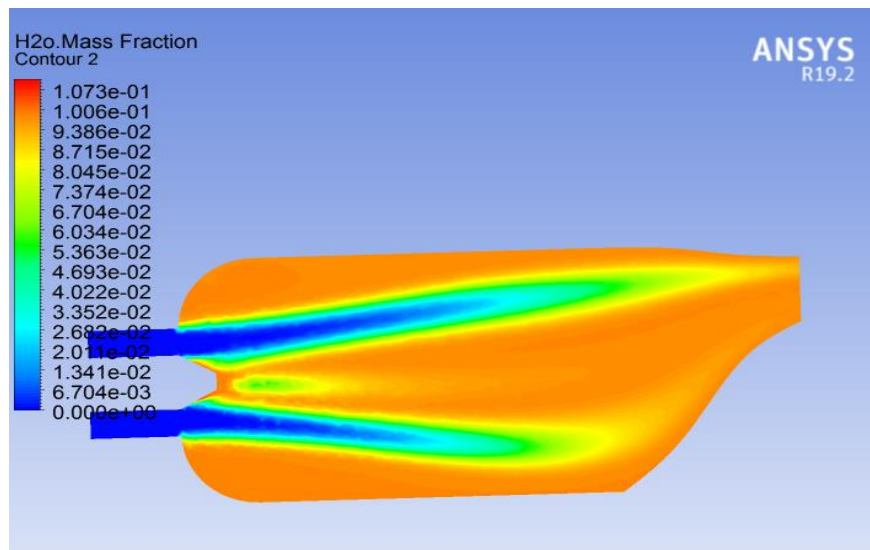


Figure 3. Mass Fraction of H₂O

Similar behaviour has been shown by the CO₂ with zero initial mass fraction at the inlet to a final composition of 0.174 as can be seen by the orange region in figure 4.

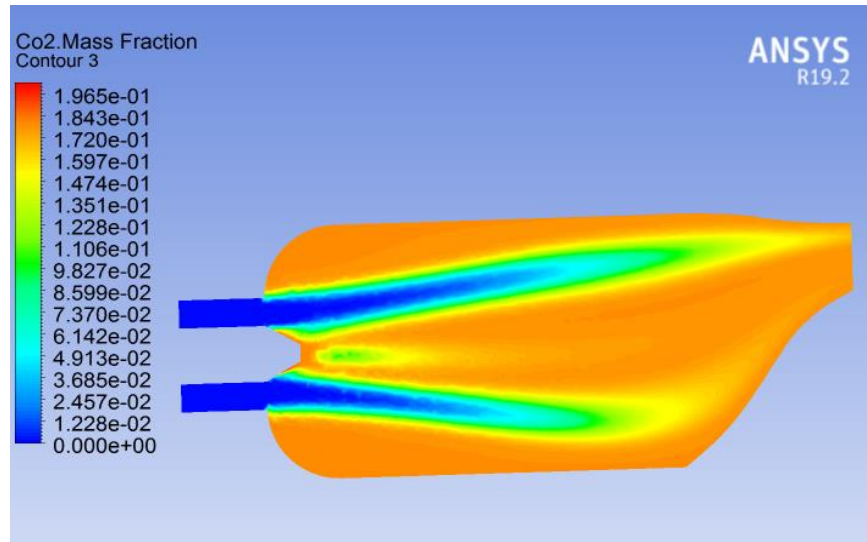


Figure 4. Mass Fraction of CO₂.

Figure 5. reveals the O₂ mass fraction distribution along the can chamber. The red region shows maximum O₂ composition at the inlet of the chamber. After complete combustion, O₂ is consumed to form products and its final composition is of almost zero shown by the blue region.

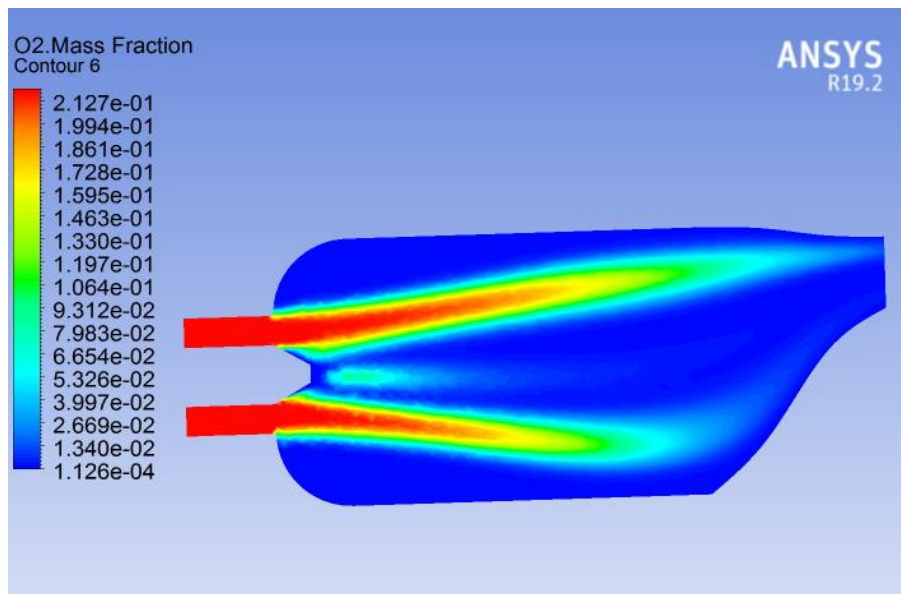


Figure 5. Mass Fraction of O₂

Similar behaviour can be seen for fuel C_3H_8 . After complete combustion, C_3H_8 is consumed to form products and its final composition is almost zero shown by the blue region.

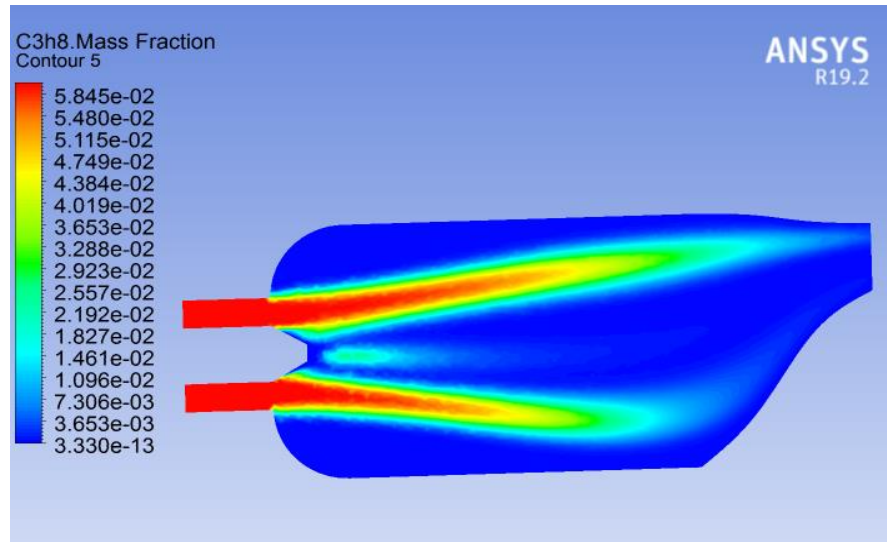


Figure 6. Mass Fraction of C_3H_8 .

3.2.1. Lean Condition for Propane ($\phi = 0.75$)

a) Adiabatic Flame Temperature

Figure 7 demonstrates the temperature distribution along the can chamber. It starts with the set gas mixture temperature of 298 K as seen in the blue region. The colour change demonstrates the increase of temperature as gasses are heated to reach ignition temperature. The red area depicts the final flame temperature of 1957 K at the stoichiometric condition.

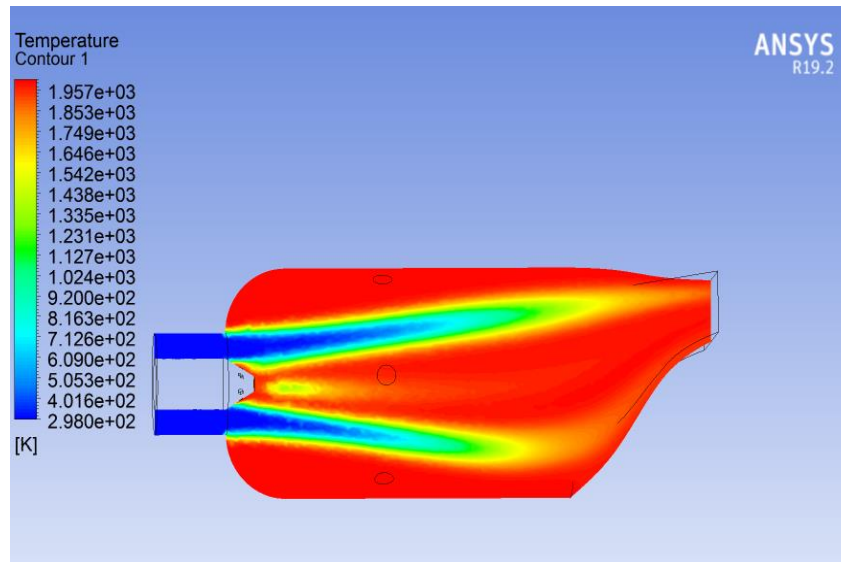


Figure7. Lean ($\phi = 0.75$) Adiabatic Flame Temperature

b) Mole fractions of products at the combustor exit plane

| H₂O(CFD) | CO₂(CFD) | O₂(CFD) | N₂(CFD) |
|----------------------------|----------------------------|---------------------------|---------------------------|
| 0.115 | 0.086 | 0.053 | 0.744 |

Table 3. Mole Fraction of Products at Exit Plane (Lean Mixture)

c) Mass fractions of products at the combustor exit plane

| H₂O(CFD) | CO₂(CFD) | O₂(CFD) | N₂(CFD) |
|----------------------------|----------------------------|---------------------------|---------------------------|
| 0.0729 | 0.134 | 0.061 | 0.732 |

Table 4. Mass Fraction of Products at Exit Plane (Lean Mixture)

The mass fraction distributions of each species are obtained from the CFD analysis along the cross-section of the can chamber for the lean reaction.

Figure 8. demonstrates the H₂O mass fraction distribution along the can chamber of lean reaction. The blue region shows zero H₂O composition at the inlet and as the reaction proceeds, H₂O is formed and its composition is increased. After complete combustion, the final mass fraction composition of H₂O is shown by the orange region to be of about 0.0729.

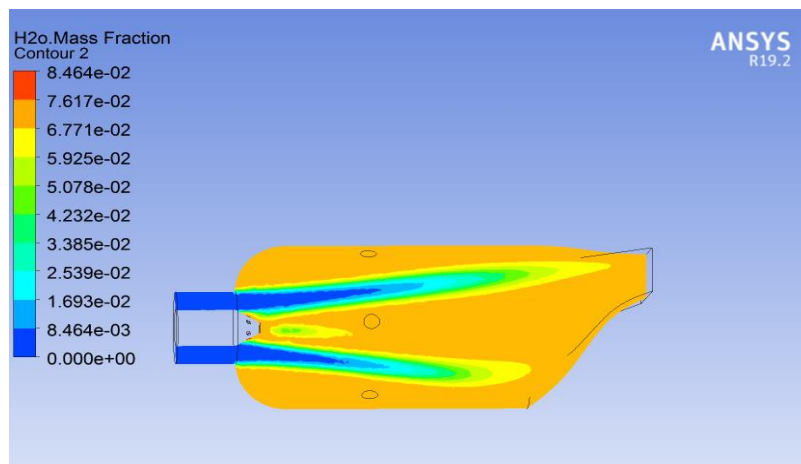


Figure 8. Mass Fraction of H₂O (lean)

Similar behaviour has been shown by the CO₂ with zero initial mass fraction at the inlet to a final composition of 0.134 as can be seen by the orange region in figure 9.

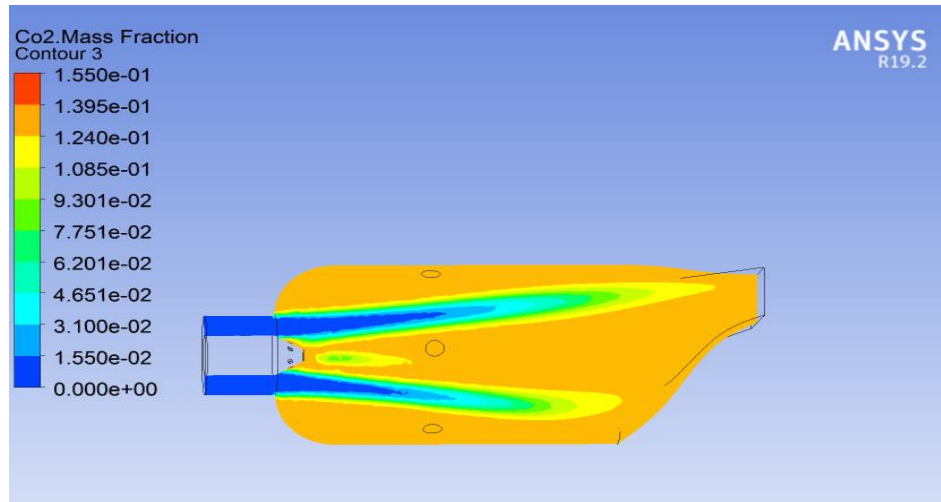


Figure 9. Mass Fraction of CO₂.

Figure 10. reveals the O₂ mass fraction distribution along the can chamber. The red region shows maximum O₂ composition at the inlet of the chamber. After complete combustion, most of O₂ is consumed to form products but as seen by the light blue region at the exit, there is an unconsumed part of O₂ in the final composition of about 0.061 at the exit.

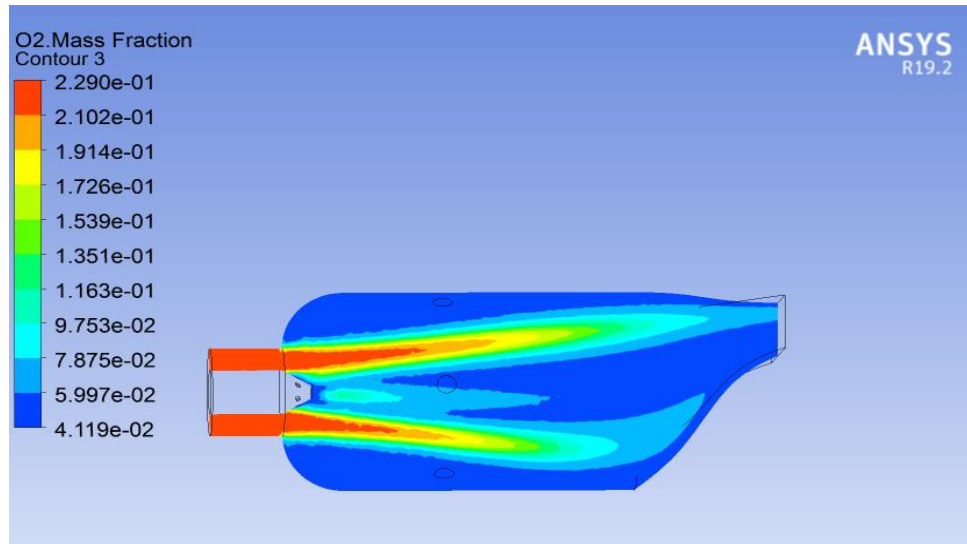


Figure 10. Mass Fraction of O₂.

Similar behaviour can be seen for fuel C_3H_8 . After complete combustion, C_3H_8 is consumed to form products and its final composition is almost zero shown by the blue region.

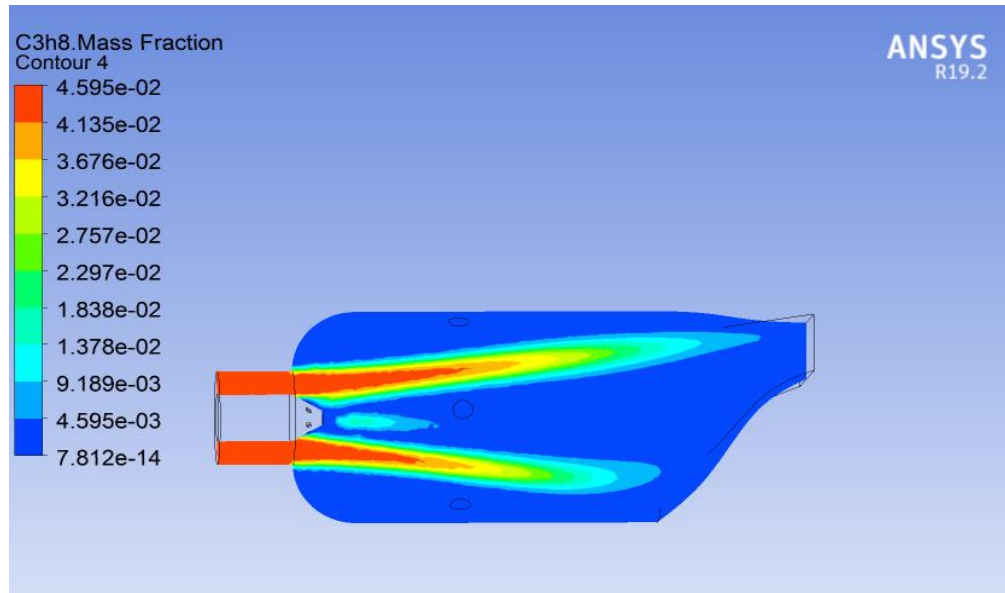


Figure 11. Mass Fraction of C3H8.

3.2. Comparison Analysis

3.2.1. Adiabatic Flame Temperature

The table below displays both the numerical and analytical calculation for final adiabatic flame temperature of the stoichiometric and lean mixture calculations. The percent error between the two for both cases are calculated with the following equation.

$$\text{Percent Error} = \left| \frac{\text{approximation} - \text{exact}}{\text{exact}} \right| * 100\%$$

| Stoichiometric Mixture | | Lean Mixture ($\phi = 0.75$) | |
|------------------------|------------------------|--------------------------------|------------------------|
| T_f (K) (CFD) | T_f (K) (Analytical) | T_f (K) (CFD) | T_f (K) (Analytical) |
| 2376 | 2393.4 | 1957 | 1981.6 |

Table 5. Adiabatic Flame Temperature

$$\text{Percent Error} = \left| \frac{\text{approximation} - \text{exact}}{\text{exact}} \right| * 100\%$$

Stoichiometric Mixture percent error:

$$T_f \text{ stoich percent error} = \left| \frac{2376 - 2393.4}{2393.4} \right| * 100\% = 0.727\%$$

Lean Mixture ($\phi=0.75$) percent error

$$T_f \text{ Lean percent error} = \left| \frac{1957 - 1981.6}{1981.6} \right| * 100\% = 1.24\%$$

3.2.2. Mole Fraction of Products at Exit Plane

| H₂O (CFD) | H₂O (Analytical) | CO₂ (CFD) | CO₂ Analytical | N₂ (CFD) | N₂ Analytical |
|---------------------------------------|--|---------------------------------------|--|--------------------------------------|---|
| 0.149 | 0.155 | 0.112 | 0.116 | 0.729 | 0.728 |

Table 6. Mole Fraction of Products at Exit Plane (Stoichiometric Condition)

Table 6. above demonstrate the results mole fraction of the product species for the stoichiometric reaction for the analytical and numerical calculations. Using the percent error formula in previous section, the error calculations for each of the species are listed below.

Stoichiometric percent error H₂O mole fraction: 3.9%

Stoichiometric percent error CO₂ mole fraction: 3.4%

Stoichiometric percent error N₂ mole fraction: 0.14%

| H₂O (CFD) | H₂O Analytical | CO₂ (CFD) | CO₂ Analytical | O₂ (CFD) | O₂ Analytical | N₂ (CFD) | N₂ Analytical |
|---------------------------------------|--|---------------------------------------|--|--------------------------------------|---|--------------------------------------|---|
| 0.115 | 0.118 | 0.086 | 0.088 | 0.053 | 0.050 | 0.744 | 0.743 |

Table 7. Mole Fraction of Products at Exit Plane (Lean Condition)

Table 7. above demonstrate the results mole fraction of the product species for the lean reaction for the analytical and numerical calculations. Using the percent error formula in previous section, the error calculations for each of the species are listed below.

Lean percent error H₂O mole fraction: 2.5%

Lean percent error CO₂ mole fraction: 2.3%

Lean percent error N₂ mole fraction: 0.13%

Lean percent error O₂ mole fraction: 6%

3.2.3. Mass Fraction of Products at Exit Plane

| H₂O (CFD) | H₂O Analytical | CO₂ (CFD) | CO₂ Analytical | N₂ (CFD) | N₂ Analytical |
|---------------------------------|--------------------------------------|---------------------------------|--------------------------------------|--------------------------------|-------------------------------------|
| 0.095 | 0.098 | 0.174 | 0.181 | 0.720 | 0.720 |

Table 8. Mass Fraction of Products at Exit Plane (Stoichiometric Condition)

Table 8. above demonstrate the results mass fraction of the product species for the stoichiometric reaction for the analytical and numerical calculations. Using the percent error formula in previous section, the error calculations for each of the species are listed below.

Stoichiometric percent error H₂O mole fraction: 2.8%

Stoichiometric percent error CO₂ mole fraction: 3.9%

Stoichiometric percent error N₂ mole fraction: 0%

| H₂O (CFD) | H₂O Analytical | CO₂ (CFD) | CO₂ Analytical | O₂ (CFD) | O₂ Analytical | N₂ (CFD) | N₂ Analytical |
|---------------------------------|--------------------------------------|---------------------------------|--------------------------------------|--------------------------------|-------------------------------------|--------------------------------|-------------------------------------|
| 0.0729 | 0.075 | 0.134 | 0.137 | 0.061 | 0.056 | 0.732 | 0.731 |

Table 9. Mass Fraction of Products at Exit Plane (Lean Condition)

Table 9. above demonstrate the results mass fraction of the product species for the lean reaction for the analytical and numerical calculations. Using the percent error formula in previous section, the error calculations for each of the species are listed below.

Lean percent error H₂O mole fraction: 2.8%

Lean percent error CO₂ mole fraction: 2.2%

Lean percent error N₂ mole fraction: 0.13%

Lean percent error O₂ mole fraction: 8.9%

As seen above, water and oxygen demonstrate to have the highest percent error for both mole and mass fraction at the exit for the lean reaction. The difference between the analytical and numerical solution for these product species are stilling within less than 10% margin of error.

4. Discussion and Conclusions

The CFD analysis of propane with air was performed in a can combustor for stoichiometric and lean condition ($\phi = 0.75$) to analyze the adiabatic flame temperature along with the mole and mass fraction of different species. The same study was done analytically and comparison with the numerical results was presented in the paper. It was observed that the numerically calculated adiabatic flame temperature of the lean mixture was about 1957 K compared to 2376 K for that of the stoichiometric mixture. The lower flame temperature for the lean mixture was because of the excess air present in the air-fuel mixture that absorbed the heat from the combustion flame, resulting in a decrease in the temperature of the flame. Both the CFD results were compared with the calculated analytical values, and it was found that all the results were in good agreement with the analytical data. Further, the mole and mass fraction of products were determined and it was discovered that in the lean mixture there was an unconsumed part of O₂ in the products. All the results obtained were in good agreement with the analytical mole and mass fraction.

5. References

- [1] Bringing the Gas Appliance Community Together, <http://www.asge-national.org/>
- [2] Principles of Combustion. K.K. Kuo, 2nd edition.