FUNDAMENTALS OF COMBUSTION (ME608)

Course Project

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Answer 1

The following quantities are given:

1. Ethane (C_2H_6) & Air
2. $\phi = 0.6$
3. Diameter $= 0.03$ m
4. Ti $= 1000$ K
5. Pi $= 1$ atm
6. $\dot{m} = 0.2$ kg/s
7. $\epsilon = 0.8$
8. $\Delta H_c = 4 \times 10^7$ J/kg
9. $C_p = 0.122 \times 10^4$ J/kg-K
10. $A_f^\star = 4.338 \times 10^8$
11. $x = 0.1$
12. $y = 1.65$
13. $E_T = 15098$
14. $m = 2$
15. $n = 6$
16. $a_{stoic} = m + n/4$

The assumptions made while using this model were:

i.   Steady state
ii. No mixing in axial direction
iii. Uniform properties perpendicular to the direction of flow
iv. Ideal frictionless flow
v.   Ideal gas behavior

The governing equations for the plug flow reactor model are:

i.   Mass conservation equation

$$\frac{d}{dx}(\rho v_x) = 0 \;\Rightarrow\; \rho v_x = c \Rightarrow \dot{m}'' = \text{constant}$$

ii. Species equation

$$\rho v_x \frac{dY_i}{dx} - \frac{d}{dx}\left[\rho D \frac{dY_i}{dx}\right] = \dot{m}_i''' \Rightarrow \dot{m}_x'' \frac{dY_i}{dx} = \dot{m}_i'''$$

iii. Momentum equation

$$\rho v_x \frac{dv_x}{dx} + \frac{dP}{dx} = 0$$

As the pressure variation is negligible, we can ignore momentum equation.

iv.   Energy equation:

$$\dot{m}'' \frac{d}{dx}(C_p T) - \frac{d}{dx}\left(\rho D \frac{d}{dx}(C_p T)\right) = -\sum h^o_{f,i} \dot{m}'''_i$$

which can be simplified to the following equation:

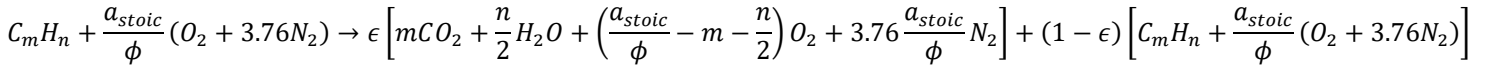$$\dot{m}'' \frac{d}{dx}(C_p T) = -\sum h^o_{f,i} \dot{m}'''_i = \dot{Q}_{chem}$$

For a single step reaction:

$$\dot{Q}_{chem} = \Delta H_c \dot{m}'''_F$$

Thus,

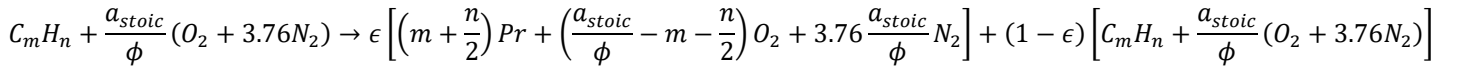$$\dot{m}'' \frac{d}{dx}(C_p T) = \Delta H_c \dot{m}'''_F$$

The general form of the combustion reaction of a hydrocarbon is

$$C_m H_n + \frac{a_{stoic}}{\phi}(O_2 + 3.76N_2) \rightarrow \epsilon\left[mCO_2 + \frac{n}{2}H_2O + \left(\frac{a_{stoic}}{\phi} - m - \frac{n}{2}\right)O_2 + 3.76\frac{a_{stoic}}{\phi}N_2\right] + (1-\epsilon)\left[C_m H_n + \frac{a_{stoic}}{\phi}(O_2 + 3.76N_2)\right]$$

To simplify the above equation, we define the product as:

$$Pr = mCO_2 + \frac{n}{2}H_2O$$

Therefore, the chemical equation takes the form:

$$C_m H_n + \frac{a_{stoic}}{\phi}(O_2 + 3.76N_2) \rightarrow \epsilon\left[\left(m + \frac{n}{2}\right)Pr + \left(\frac{a_{stoic}}{\phi} - m - \frac{n}{2}\right)O_2 + 3.76\frac{a_{stoic}}{\phi}N_2\right] + (1-\epsilon)\left[C_m H_n + \frac{a_{stoic}}{\phi}(O_2 + 3.76N_2)\right]$$

Using our Plug Flow Reactor model,

$$\dot{m}'' = constant \Rightarrow \dot{m}/A = constant$$
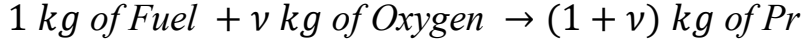
$$\frac{dY_F}{dx} = -\frac{A}{\dot{m}}|\dot{m}'''_F|$$

$$\frac{dY_{Ox}}{dx} = -\frac{A}{\dot{m}}|\dot{m}'''_{Ox}|$$

$$\frac{dY_{Pr}}{dx} = \frac{A}{\dot{m}}|\dot{m}'''_{Pr}|$$

$$\frac{dY_{N_2}}{dx} = 0 \quad (\text{As } N_2 \text{ is inert})$$

$$\frac{d(C_p T)}{dx} = \frac{A}{\dot{m}} \Delta H_c \dot{m}_F'''$$

For a stoichiometric reaction,

$$1 \; kg \; of \; Fuel \; + v \; kg \; of \; Oxygen \; \rightarrow (1+v) \; kg \; of \; Pr$$

Where v is defined as:

$$v = \frac{M_{O_2}}{M_F} a_{stoic} = \frac{M_{O_2}}{M_F} \left(m + \frac{n}{4} \right)$$

$$v = 3.733$$

Thus, we can relate the $\dot{m}_{Ox}'''$ and $\dot{m}_{Pr}'''$ with $\dot{m}_F'''$

$$\dot{m}_{Ox}''' = v \, \dot{m}_F'''$$

$$\dot{m}_{Pr}''' = -(1+v) \, \dot{m}_F'''$$

The final coupled system of first order linear differential equation that we need to solve is:

$$\frac{dY_F}{dx} = -\frac{A}{\dot{m}} |\dot{m}_F'''|$$

$$\frac{d}{dx}\left(\frac{Y_{Ox}}{v} \right) = -\frac{A}{\dot{m}} |\dot{m}_F'''|$$

$$\frac{d}{dx}\left(\frac{Y_{Pr}}{1+v} \right) = \frac{A}{\dot{m}} |\dot{m}_F'''|$$

$$\frac{d}{dx}(C_p T) = \frac{A}{\dot{m}} \Delta H_c |\dot{m}_F'''|$$

Since the following quantities are not varying with space, we conclude they are constant with space, and thus are equal to the initial and final values.

$$\frac{d}{dx}\left[Y_F - \frac{Y_{Ox}}{v} \right] = 0$$

$$\frac{d}{dx}\left[Y_F + \frac{Y_{Pr}}{1+v} \right] = 0$$

$$\frac{d}{dx}\left[C_p T + \Delta H_c \, Y_F \right] = 0$$

It is given that the volumetric mass flow rate depends on various quantities and varies as follows:

$$\dot{m}_F''' = A_F^* \, \rho_{mix}^{(x+y)} \, e^{\left(\frac{-E_T}{T}\right)} \, Y_F^x \, Y_{O_2}^y$$

where, the density and molecular mass of the mixture is defined as follows:

$$\rho_{mix} = \frac{P M_{mix}}{R_u T}$$

$$M_{mix} = \left[\sum \frac{Y_i}{M_i}\right]^{-1}$$

Thus, the equation for volumetric mass flow rate is:

$$\dot{m}_F''' = A_F^* \left[\frac{P M_{mix}}{R_u T}\right]^{(x+y)} e^{\left(\frac{-E_T}{T}\right)} \left(Y_{F_i} - \frac{C_p(T - T_i)}{\Delta H_c}\right)^x \left(Y_{O_{2,i}} - \frac{v C_p(T - T_i)}{\Delta H_c}\right)^y$$

For the initial conditions, at x = 0:

$$M_{mix} = M_F + \frac{a_{stoic}}{\phi}\left(M_{O_2} + 3.76 M_{N_2}\right)$$

$$Y_{F,i} = \frac{M_F}{M_{mix}}$$

$$Y_{Ox,i} = \frac{a_{stoic} \, M_{Ox}}{\frac{\phi}{M_{mix}}}$$

$$Y_{N_{2,i}} = 1 - Y_{F,i} - Y_{Ox,i} - Y_{Pr,i}$$

For the final conditions, at x = L:

$$m_{mix} = (1 - \varepsilon)M_F + \varepsilon(m + n/2)M_{Pr} + \left[\frac{a_{stoic}}{\phi} - \varepsilon\left(m + \frac{n}{2}\right)\right]M_{Ox} + 3.76\frac{a_{stoic}}{\phi} M_{N_2}$$

$$Y_{F,L} = (1 - \varepsilon)\frac{M_F}{M_{mix}}$$

$$Y_{Ox,L} = \left[\frac{a_{stoic}}{\phi} - \varepsilon\left(m + \frac{n}{2}\right)\right]\frac{M_{Ox}}{M_{mix}}$$

$$Y_{Pr,L} = \varepsilon(m + n/2)\frac{M_{Pr}}{M_{mix}}$$

$$Y_{N_2,L} = Y_{N_2,i}$$

Thus, the final equation that we need to solve to get the rest of the quantities is:

$$\frac{dT}{dx} = \frac{A}{\dot{m}} \frac{\Delta H_c}{C_p} \dot{m}_F'''$$

Using Euler's marching integration technique,

$$T_{x+\Delta x} = T_x + \Delta x \frac{A\Delta H_c}{\dot{m}C_p} \dot{m}_F'''$$

To estimate the length required for the reaction to go to 80% completion, we use the following interpolation formula:

$$\frac{L - x_{old}}{x_{new} - x_{old}} = \frac{Y_{Pr,L} - Y_{Pr,old}}{Y_{Pr,new} - Y_{Pr,old}}$$

Which gives us the length, L, required as:

$$L = x_{old} + (x_{new} - x_{old}) \left[\frac{Y_{Pr,L} - Y_{Pr,old}}{Y_{Pr,new} - Y_{Pr,old}} \right]$$

RESULTS:

Upon solving the above system of coupled ordinary linear differential equations, we found out that the length required will be: 0.7592664290402671 meters ≈ 0.759 meters.

We solved the system using different spatial step sizes, and the observations are listed below:

Step size(m)	Iterations	Length Required(m)
0.5	4	1.51274
0.1	10	0.95102
0.05	18	0.86526
0.01	79	0.78319
0.005	155	0.77144
0.001	762	0.76173
0.0005	1522	0.76050
0.0001	7596	0.75951
0.00005	15188	0.75939
0.00001	75929	0.75929
0.000005	151856	0.75928
0.000001	759267	0.75927

We can see that the length converges to 0.7592 meters. Thus, we can deduce that the length required does not depend on the step size. The variation of different quantities with respect to the length of the reactor is shown in the following plots.
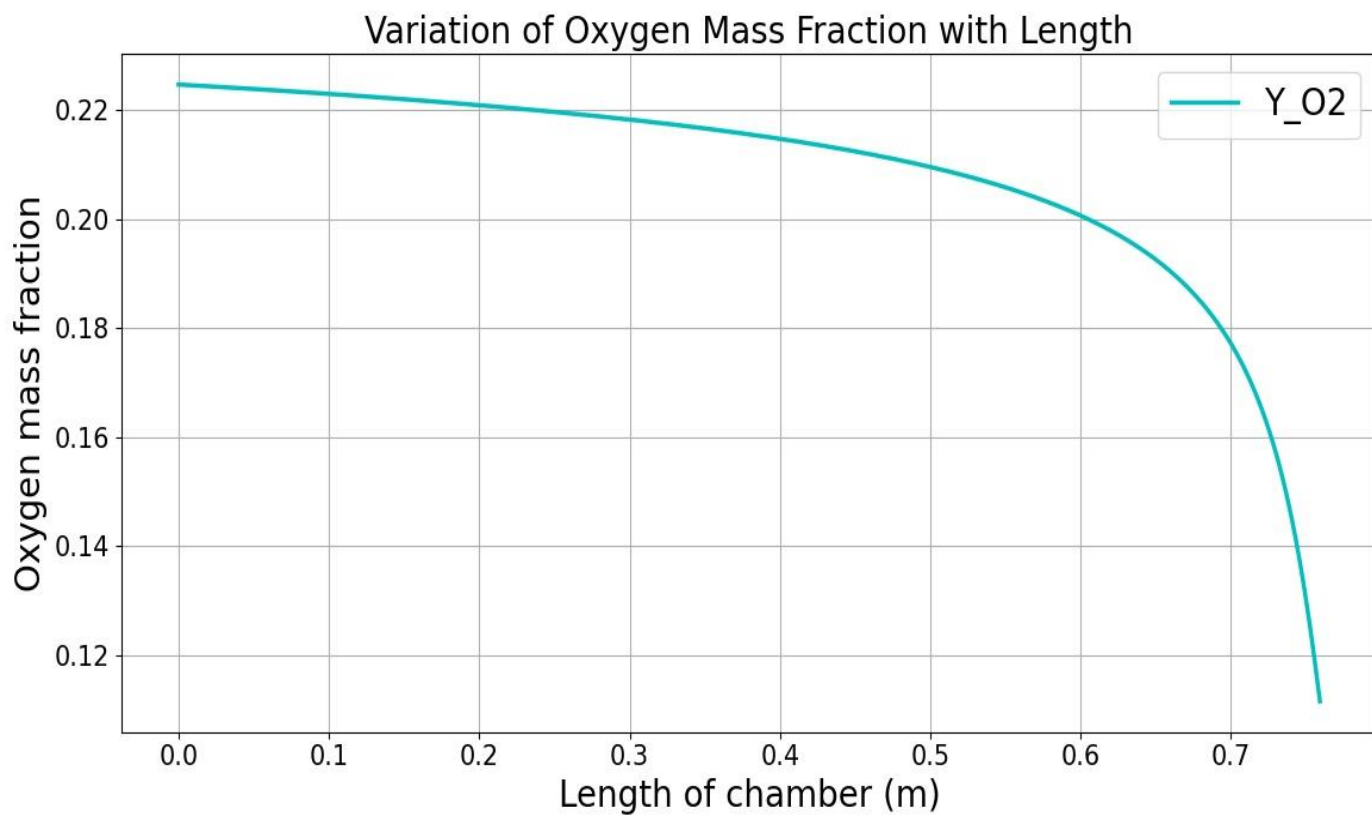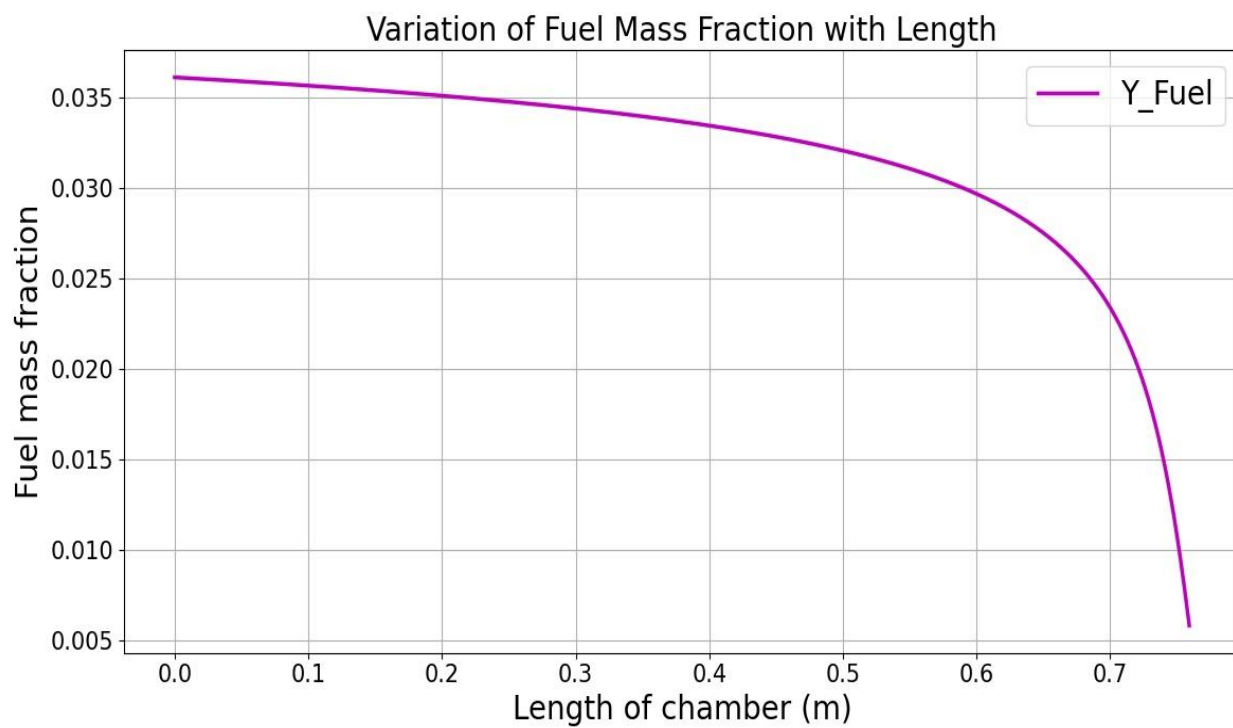All the plots are plotted with $\Delta x = 10^{-6}$.
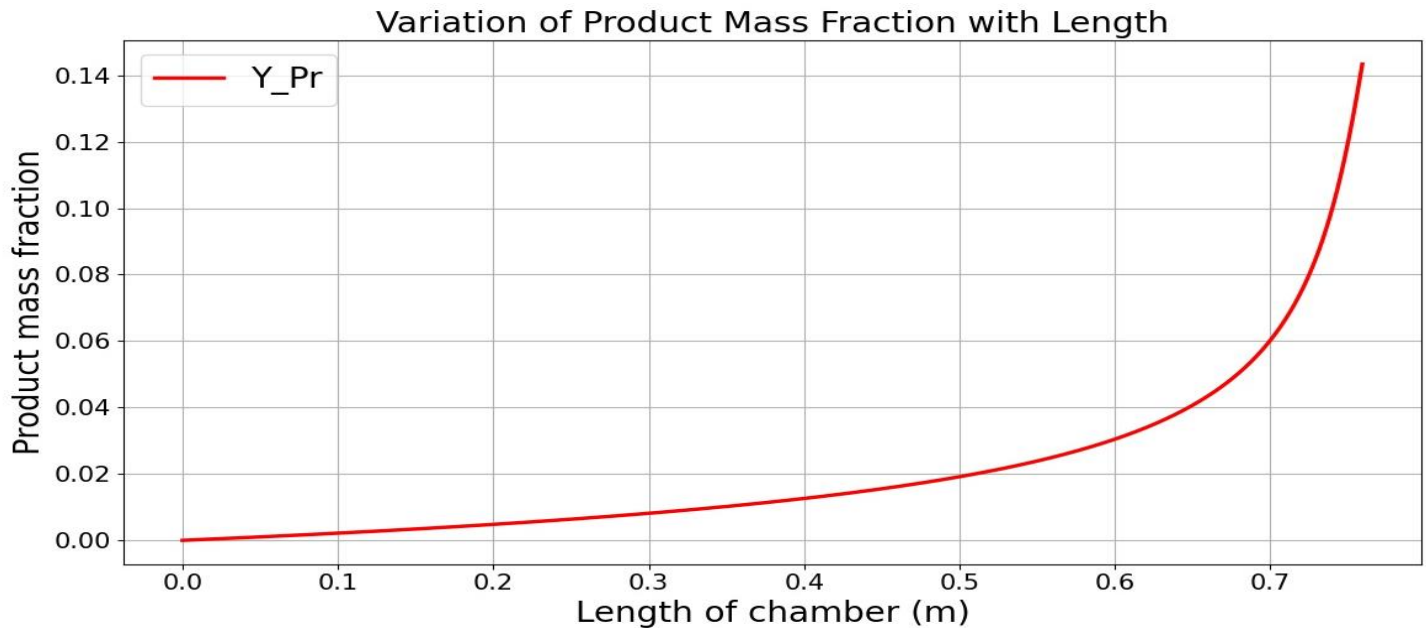
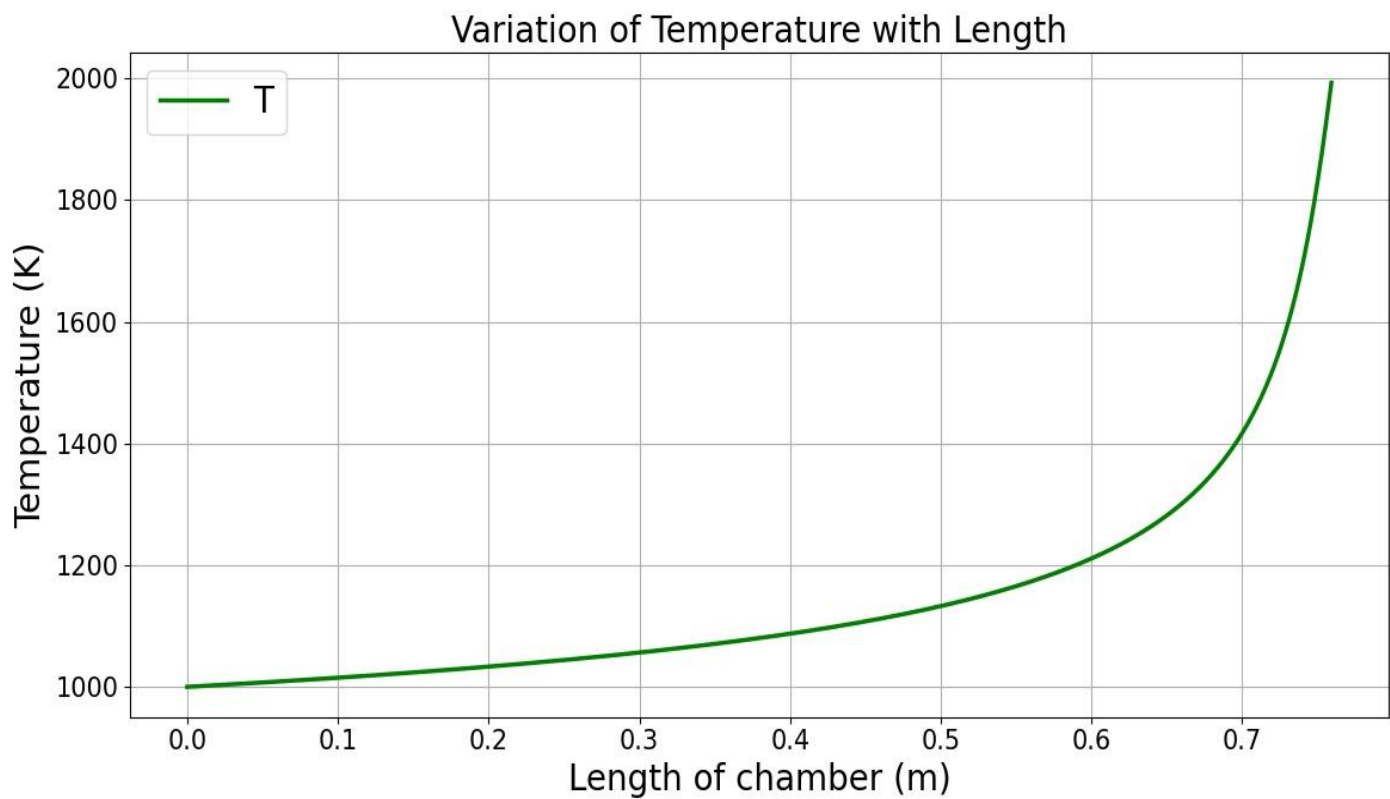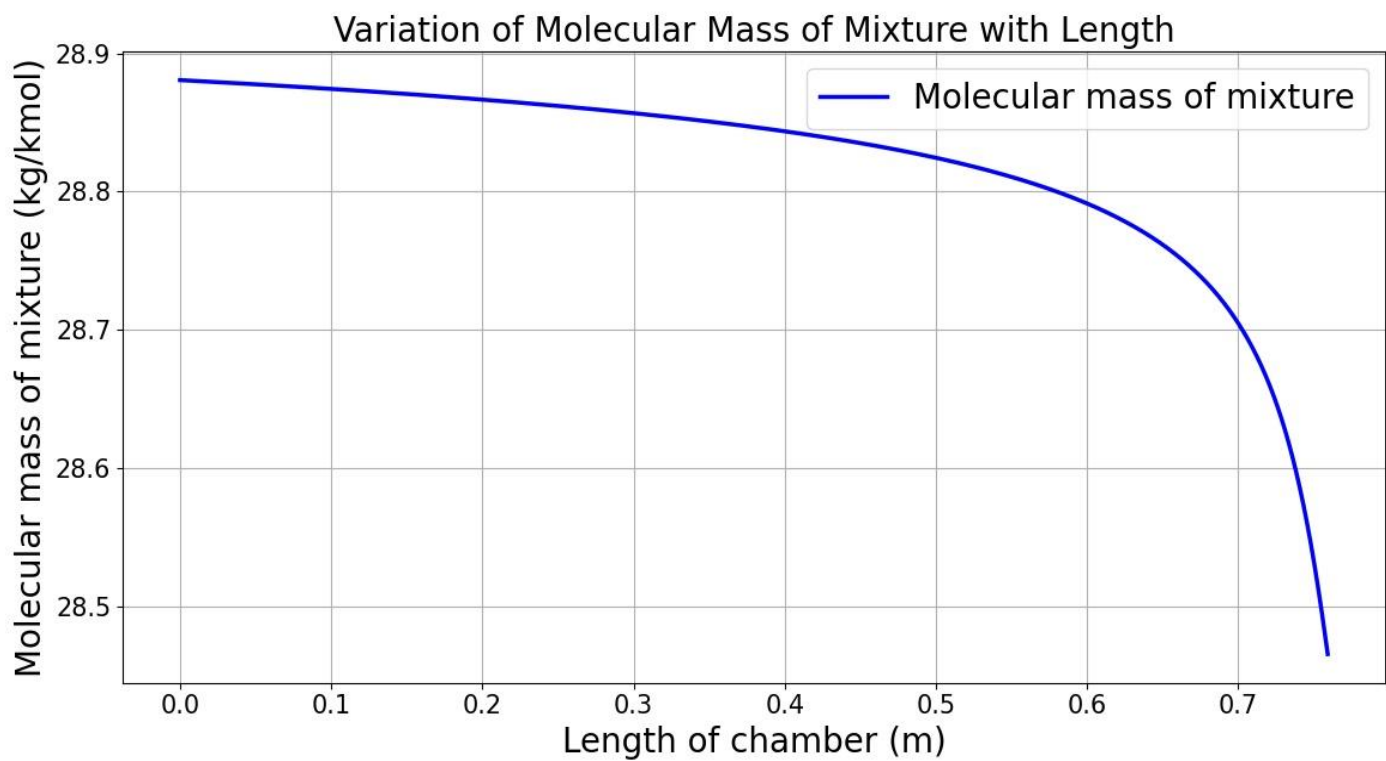*Figure 1*

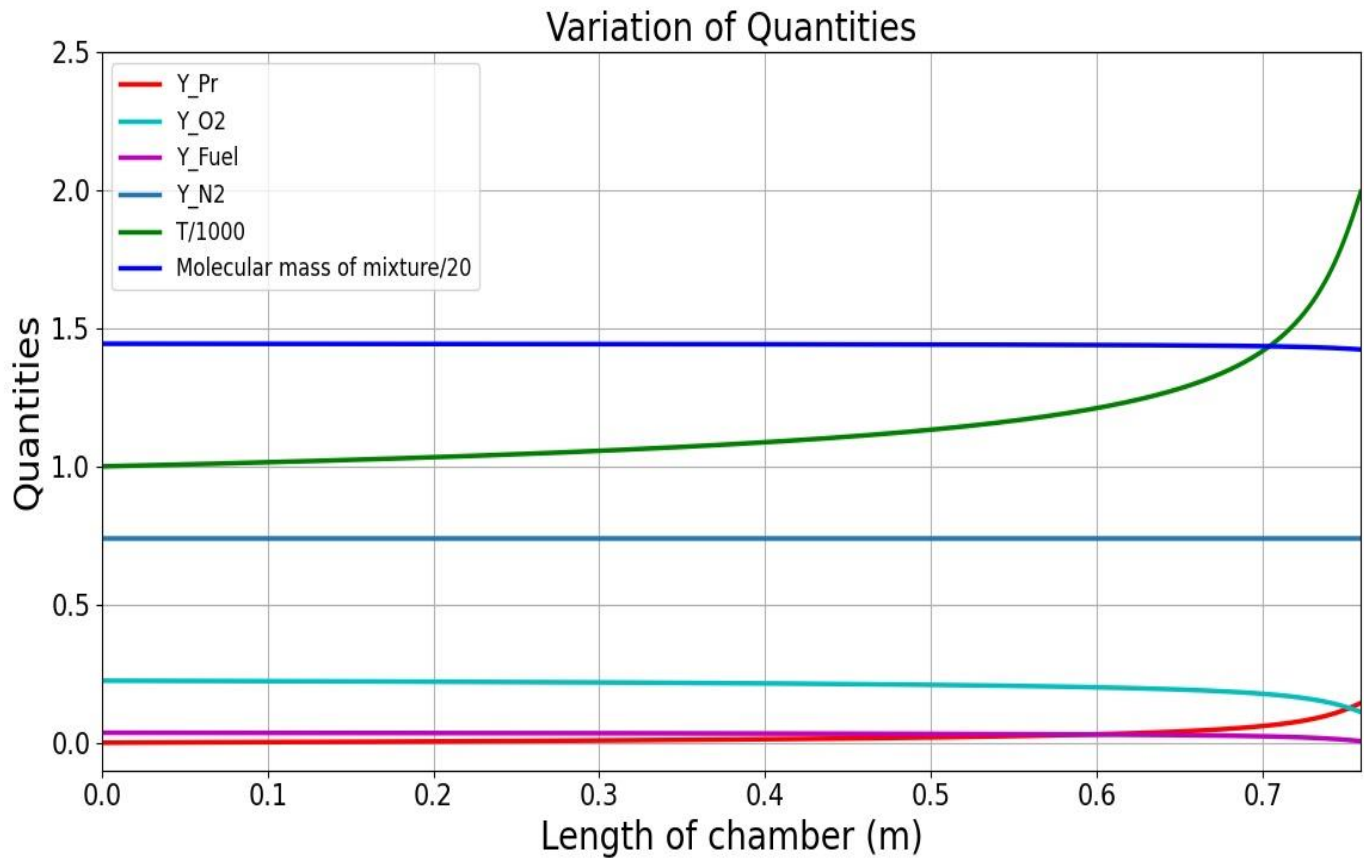*Figure 2*

Figure 3

Figure 4

Figure 5

Figure 6

INTERPRETATIONS:

- Since all the equations are first-order, ordinary linear differential equations, the general solutions are exponential, that is evident in the plotted graphs. The quantities vary as an exponential function of the length of the reactor.
- Quantities like the mass fraction of fuel, mass fraction of Oxygen, and molecular mass of fuel decrease over time as they are consumed in the reaction while product mass fraction increases as it is produced. Temperature also increase as a result of the chemical energy being released from the reaction.
- In the final graph, the mass fraction of N_2 stays constant as it is an inert component and stays unreacted.

CONCLUSIONS/COMMENTS:

- There were some contradictions between the calculated and predicted output as the total mass of the mixture was decreasing. It was concluded that there must have been some issues with the equations as the code was not wrong and multiple debugging sessions were performed to make sure that there is nothing wrong with the code. The solution obtained from the code is treated to be correct.

- To further check the credibility of the program, the following investigation was performed:
  - o In order to check the change in mass of the mixture, the calculation of mass fraction of N_2, i.e., Y_{N_2} was carried out two different methods.
    - $Y_{N_2,new} = Y_{N_2,i}$, at each updating step, the new mass fraction of N_2, $Y_{N_2,new}$ is taken to be the initial mass fraction of N_2, $Y_{N_2,i}$. This is done with the thought that since the nitrogen is inert, thus, its mass fraction remains constant. If we follow this thought, we end up getting $Y_{Total,f} = 0.9642$, wherein, it should sum up to 1, as the sum of mass fractions of all the elements adds up to one.
    - If we fix $Y_{Total,f} = 1.0$, which is correct, and then calculating Y_{N_2} as
    $$Y_{N_2,f} = 1 - Y_{F,f} - Y_{O_2,f} - Y_{Pr,f}$$
    we end up getting $Y_{N_2,f}$ as 0.7750, where in reality it should be 0.7392
- In the following graphs, the dot represents the quantities calculates using the formulas given, and we can observe that they do not match with the predicted values.
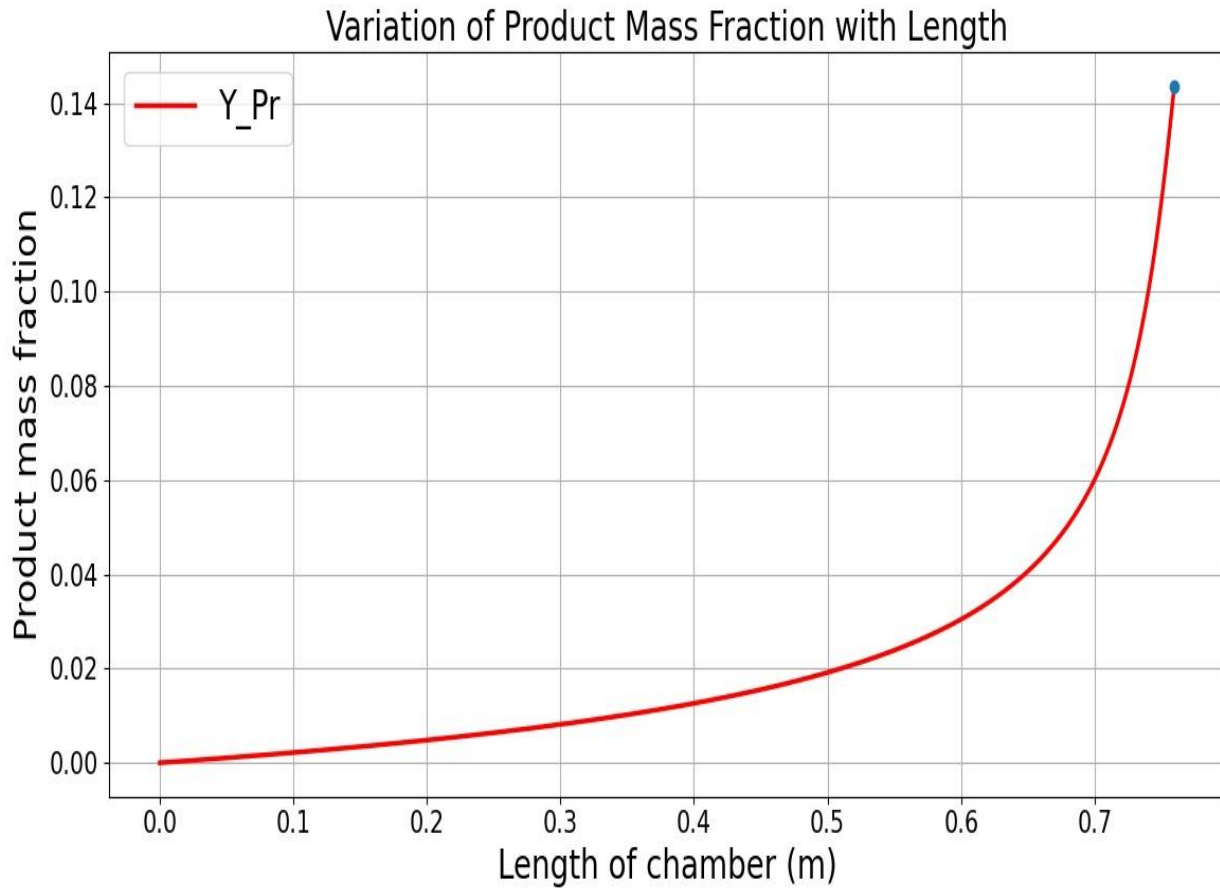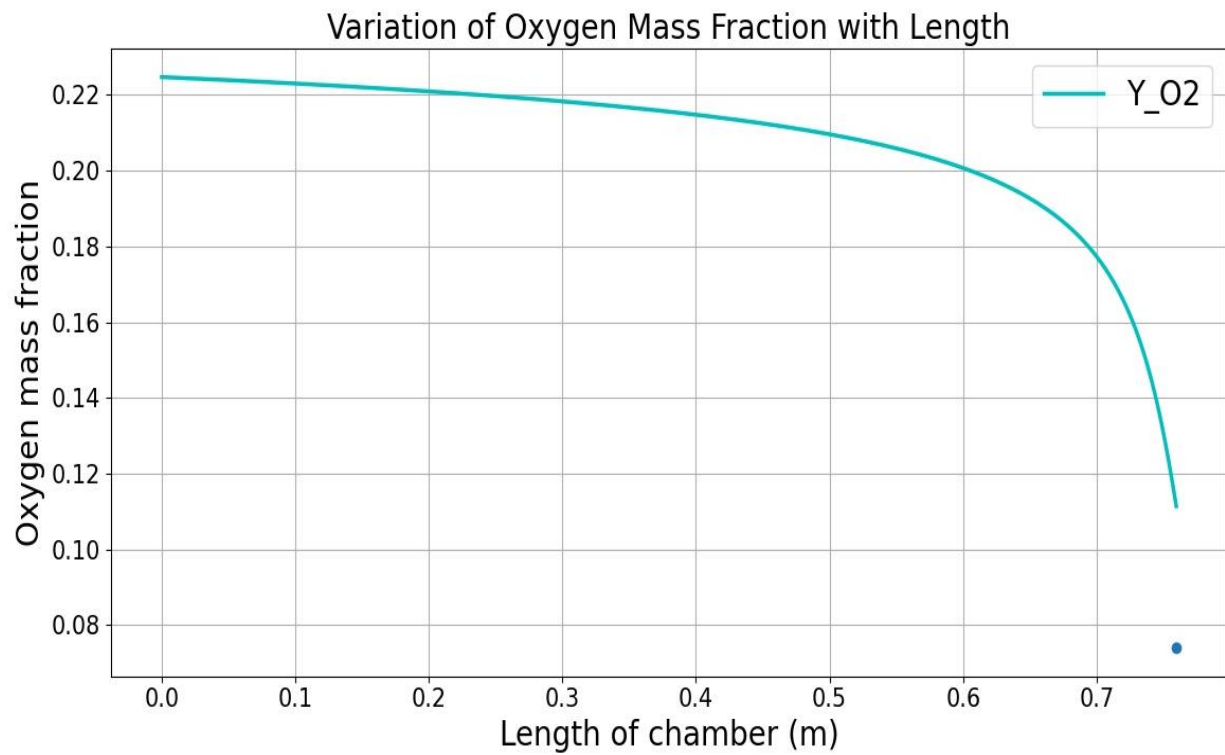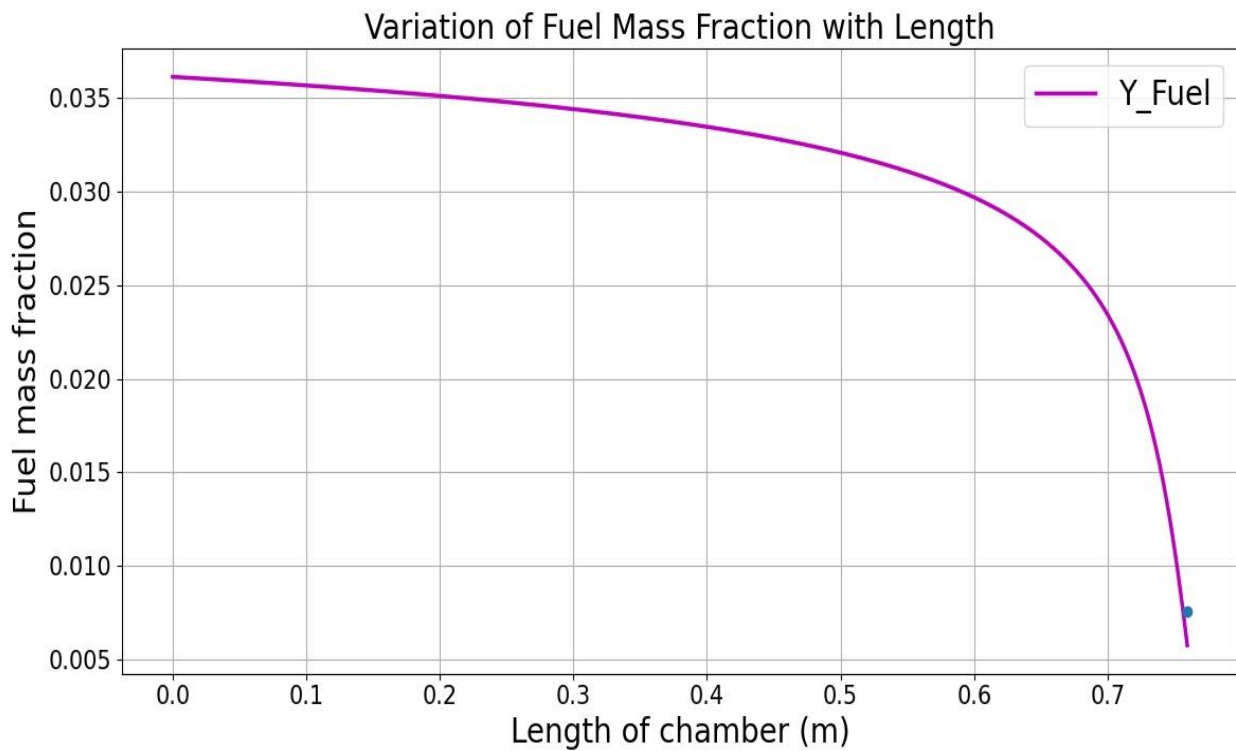

Figure 7

Figure 8

Figure 9

- The length of the reactor required for taking the reaction to 80% completion is ~0.76 meters.
- The final temperature reached is: 1994.756 K

Answer 2

The following quantities are given:
1. Propane (C_3H_8)
2. $\phi = 1.0$
3. Diameter = 0.08 m
4. T1 = 298 K
5. P1 = 1 atm
6. $\dot{m} = 0.1$ kg/s
7. $M_{mix} = 29$ kg/kmol
8. $\Delta H_c = 4.65 \times 10^7$ J/kg
9. $T_{adiabatic} = 2394$ K
10. $C_p = 0.1230 \times 10^4$ J/kg-K
11. $A_f^\star = 4.836 \times 10^9$
12. $x = 0.1$
13. $y = 1.65$
14. $E_a/R_u = 15098$
15. $m = 3$
16. $n = 8$
17. $a_{stoic} = m + n/4$
18. $V_{CV} = \pi D^3 / 6$

Assumptions made:

i. Perfect mixing is achieved inside the control volume
ii. The materials entering the reactor at state 1 attains the properties of state 2 instantaneously

A well stirred reactor is also known stubby plug flow reactor where the quantities are approximated as:

$$\frac{d\phi}{dx} = \frac{\phi_2 - \phi_1}{\Delta x}$$

The governing equations for the well stirred reactor model are:

i. Mass conservation equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v_x) = 0 \Rightarrow \rho v_x = c \Rightarrow \dot{m}'' = constant$$

ii.   Species equation

$$\rho v_x \frac{dY_i}{dx} - \frac{d}{dx}\left[\rho D \frac{dY_i}{dx}\right] = \dot{m}_i''' \Rightarrow \dot{m}_x'' \frac{dY_i}{dx} = \dot{m}_i'''$$

$$\frac{\dot{m}}{A}\left(\frac{Y_{2,i} - Y_{1,i}}{\Delta x}\right) = \dot{m}_i'''$$

$$\dot{m}(Y_{2,i} - Y_{1,i}) = V_{CV}\dot{m}_i'''$$

iii.   Momentum equation

$$\rho v_x \frac{dv_x}{dx} = -\frac{dP}{dx} + \tau_w$$
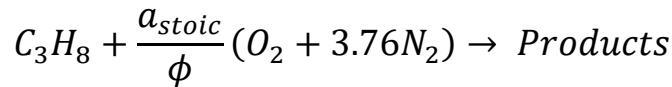
$$\rho v_x \frac{dv_x}{dx} = 0$$

iv.   Energy equation:

$$\rho v_x \frac{d}{dx}(C_pT) - \frac{d}{dx}\left(\rho D \frac{d}{dx}(C_pT)\right) = -\sum h_{f,i}^o \dot{m}_i'''$$

$$\dot{m}'' \frac{d}{dx}(C_pT) = -\sum h_{f,i}^o \dot{m}_i'''$$

$$\dot{m}'' \frac{d}{dx}(C_pT) = -\Delta H_c \dot{m}_F'''$$

$$\dot{m}C_p(T_2 - T_1) = \Delta H_c V_{CV}\dot{m}_i'''$$

Using the single-step reaction:

$$C_3H_8 + \frac{a_{stoic}}{\phi}(O_2 + 3.76N_2) \rightarrow Products$$

For the initial conditions:

$$Y_{F,i} = \frac{M_F}{M_F + \left[\frac{a_{stoic}}{\phi}\right](M_{O_2} + 3.76M_{N_2})}$$

$$Y_{Ox,i} = \frac{\left[\frac{a_{stoic}}{\phi}\right]M_{O_2}}{M_F + \left[\frac{a_{stoic}}{\phi}\right](M_{O_2} + 3.76M_{N_2})}$$

$$Y_{N_2,i} = 1 - Y_{F,i} - Y_{Ox,i}$$

For a stoichiometric reaction, ν is defined as:

$$\nu = \frac{M_{O_2}}{M_F} a_{stoic} = \frac{M_{O_2}}{M_F}\left(m + \frac{n}{4}\right)$$

$$\nu = 3.636$$

Thus, we can relate the $\dot{m}_{Ox}'''$ with $\dot{m}_F'''$

$$\dot{m}_{Ox}''' = \nu\, \dot{m}_F'''$$

The system of equations that we need to solve is:

$$Y_{F,2} - Y_{F,1} = -\frac{V_{CV}}{\dot{m}}|\dot{m}_F'''|$$

$$Y_{O_2,2} - Y_{O_2,1} = -\nu\frac{V_{CV}}{\dot{m}}|\dot{m}_F'''|$$

The above system can be further simplified using the equation for change in temperature.

$$T_2 - T_1 = \frac{\Delta H_c V_{CV}}{\dot{m} C_p}|\dot{m}_F'''| = -\frac{\Delta H_c}{C_p}\left(Y_{F,2} - Y_{F,1}\right)$$

Thus, the final coupled system of first order linear differential equation that we need to solve is:

$$Y_{F,2} = Y_{F,1} - \frac{C_p}{\Delta H_c}(T_2 - T_1)$$

$$Y_{O_2,2} = Y_{O_2,1} - \nu\frac{C_p}{\Delta H_c}(T_2 - T_1)$$

It is given that the volumetric mass flow rate depends on various quantities and varies as follows:

$$|\dot{m}_F'''| = A_F^* \, \rho_{mix}^{(x+y)} e^{\left(\frac{-E_a}{R_u T}\right)} M_F^{(1-x)} M_{O_2}^{-y} Y_F^x \, Y_{O_2}^y$$

where, the density and molecular mass of the mixture is defined as follows:

$$\rho_{mix} = \frac{P M_{mix}}{R_u T}$$

$$M_{mix} = \left[\sum \frac{Y_i}{M_i}\right]^{-1}$$

Thus, the equation for volumetric mass flow rate is:

$$|\dot{m}_F'''| = A_F^* \left[\frac{PM_{mix}}{R_uT}\right]^{(x+y)} e^{\left(\frac{-E_a}{R_uT}\right)} M_F^{(1-x)} \left(Y_{F_i} - \frac{C_p(T-T_i)}{\Delta H_c}\right)^x M_{O_2}^{-y} \left(Y_{O_{2,i}} - \frac{C_p(T-T_i)}{\Delta H_c}\right)^y$$

Thus, the final temperature can be now determined using the following equation:

$$T_2 - T_1 = \frac{\Delta H_c V_{CV}}{\dot{m}C_p}|\dot{m}_F'''| = -\frac{\Delta H_c}{C_p}(Y_{F,2} - Y_{F,1})$$

$$T_2 = T_1 + \frac{\Delta H_c V_{CV}}{C_p\dot{m}}|\dot{m}_F'''|$$

$$T_2 = T_1 + \frac{\Delta H_c V_{CV}}{C_p\dot{m}} A_F^* \left[\frac{PM_{mix}}{R_uT_2}\right]^{(x+y)} e^{\left(\frac{-E_a}{R_uT_2}\right)} M_F^{(1-x)} \left(Y_{F_1} - \frac{C_p(T_2-T_1)}{\Delta H_c}\right)^x M_{O_2}^{-y} \left(Y_{O_{2,1}} - \frac{C_p(T_2-T_1)}{\Delta H_c}\right)^y$$

The above equation is a transcendental equation and can be solved using any iterative solver for different values of the parameters $\dot{m}, \phi, P1, T1$ and D.

Plotting the RHS and LHS of the above equation to visualize the solutions. Whenever the two plots intersect, we conclude that it is a solution of the above equation.
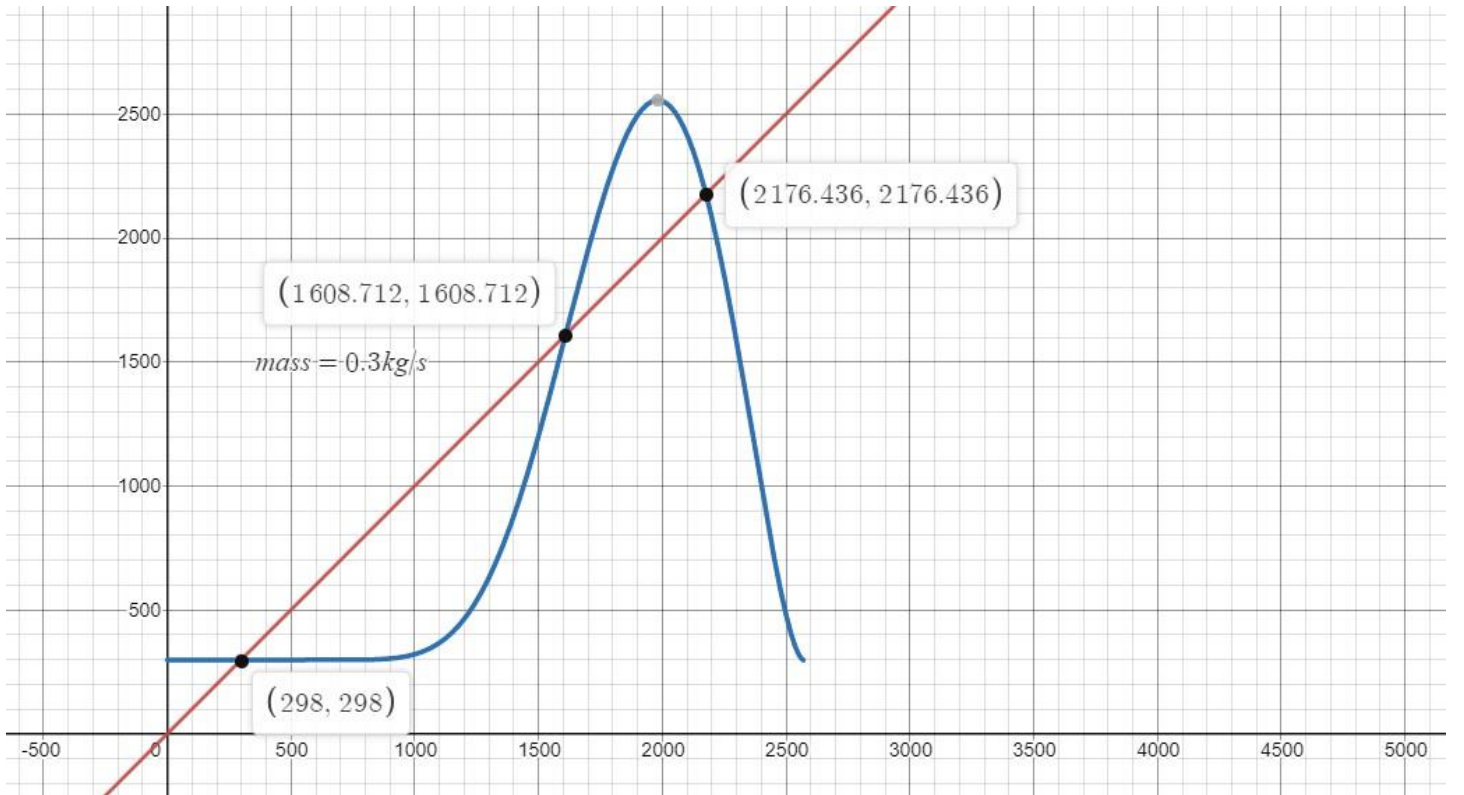

Figure 1

By observing the above graph, we can deduce that we will be getting three different solutions of the transcendental equation for each value of mass flow rate.

RESULTS:

Upon solving the transcendental equation for temperature, we get three solution corresponding to each value of mass flow rate.
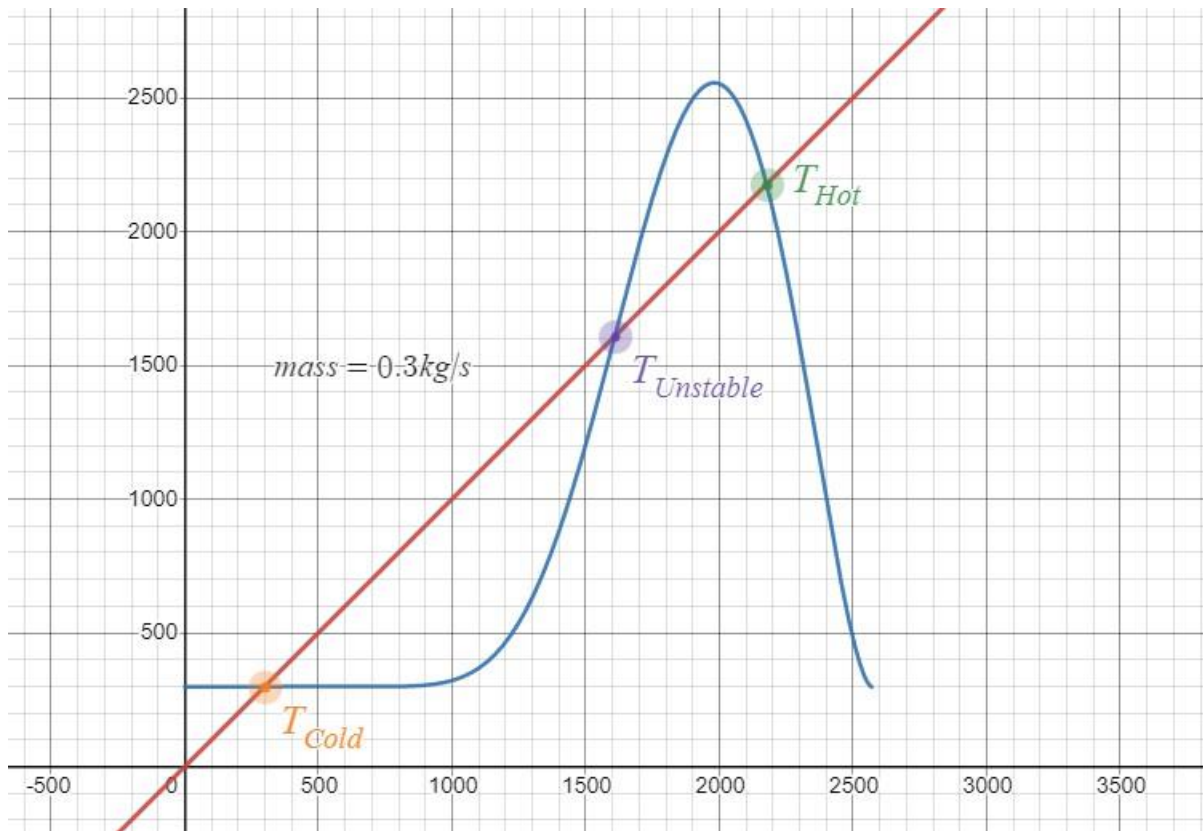

Figure 2

i. The first solution, T_{Cold} corresponds to the fuel that leaves the reactor almost unreacted. It is the trivial solution that we get for any value of mass flow rate and is equal to the initial temperature of the reactor. Therefore, it is of no use to us.

ii. The second solution, $T_{Unstable}$ corresponds to the combusted fuel that is unstable, thus, it also cannot be used to predict blow off.

iii. The third solution, T_{Hot} corresponds to the fuel that is properly combusted and can be used to predict blow off.

In the following graph, we can see the variation of all the solutions with mass flow rate.
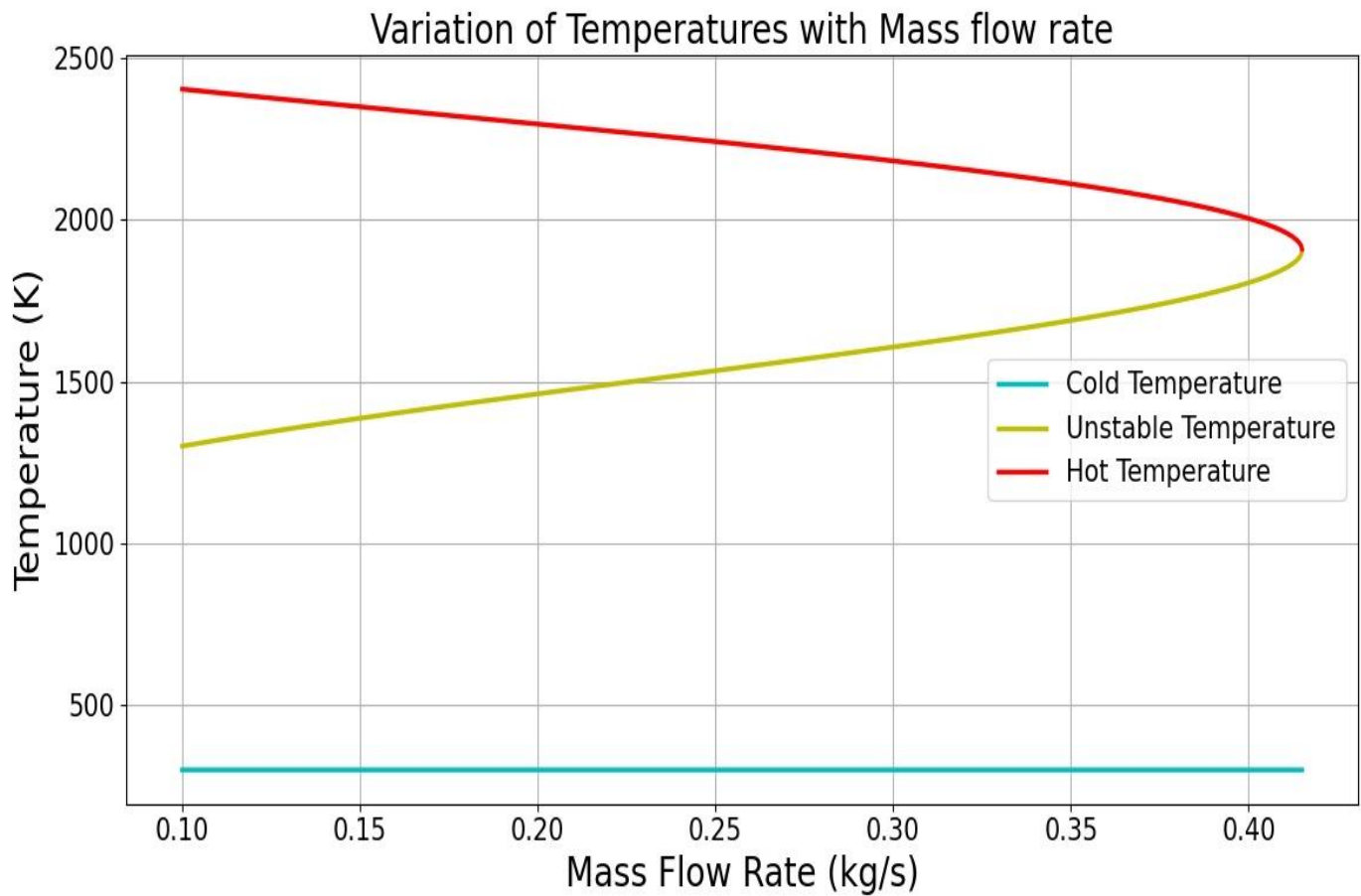
Figure 3

We can see that blow off occurs at the point where the plots of T_{Hot} and $T_{Unstable}$ intersect. The blow off takes place at a mass flow rate of 0.4151 kg/s.

The variation of exit conditions for various values of mass flow rate are shown below:
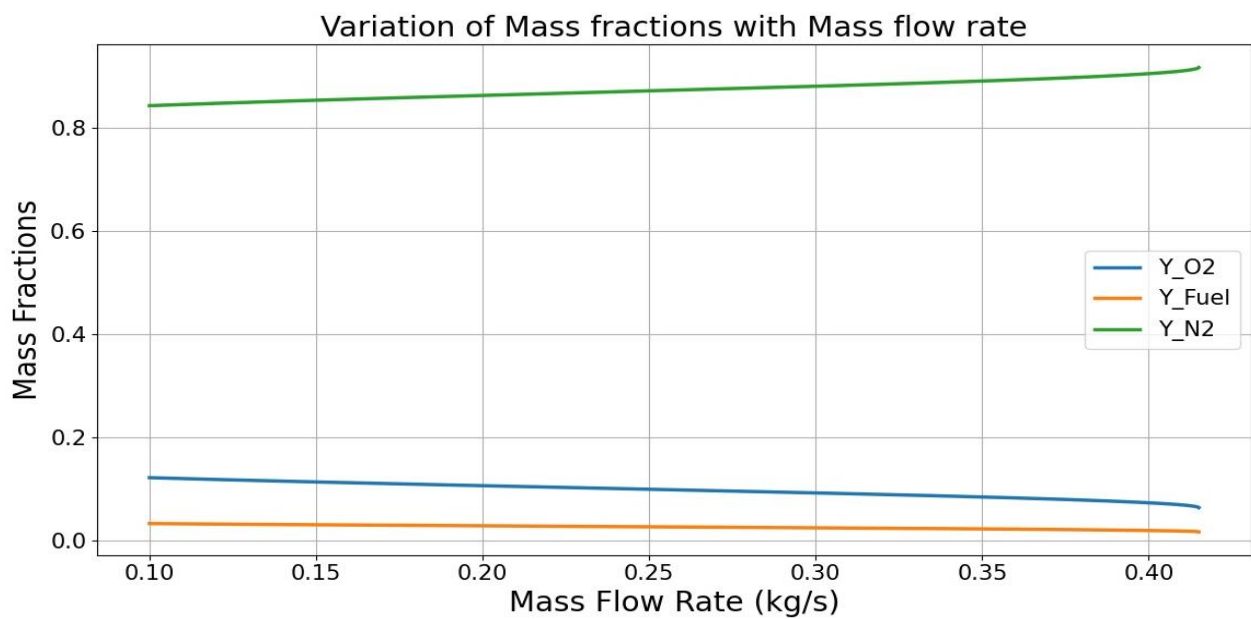

Figure 4

The exit conditions just before the blow off, i.e. at mass flow rate of 0.4150 kg/s were:

Mass fraction of fuel = 0.01779037844051396

Mass fraction of oxygen = 0.06469228523823259

Mass fraction of nitrogen = 0.9175173363212534

INTERPRETATIONS:

- Blow off condition corresponds, mathematically, to the situation where a solution for the temperature equation is not possible for a given mass flow rate and physically, to a situation when the flow speed is so high, the flame cannot be stabilized, and the flame propagate downstream and eventually extinguishes. Thus, no combustion is possible once the mass flow rate corresponding to blow off condition is attained.
- The critical mass flow rate is 0.4150 kg/s while the critical temperatures are:
  - $T_{Cold,cr}$ = 298.0 K
  - $T_{Unstable,cr}$ = 1902.84 K
  - $T_{Hot,cr}$ = 1909.608 K.
- The mass fraction for oxygen and fuel are decreasing as they are being consumed in the reaction while the mass fraction of nitrogen increases as it is an inert participant and remains unaffected throughout the process.
- In order to solve a transcendental equation of the form $T_2 = f(T_2)$, where our objective is to balance out the two sides, i.e., we have to find those T_2, such that the two sides are equal. But doing so is not possible while employing an iterative solver. Thus, we have to convert the above equation to some other function, say, $g(T_2) = T_2 - f(T_2)$ and then we have to solve for $g(T_2) = 0$, i.e., we have to find the zeroes of $g(T_2)$.
- We have developed two separate programs:
  - "Self-Coded"
    - The temperature equation is solved using Newton-Raphson method, that we developed ourselves, by calculating the expression and its derivative.
    - Newton-Raphson is an iterative solver that uses the tangent to the curves to reach to the point of global minima, which is approximated as the solution of the curve. The solver is run until the error reaches an accepted value.
    - Newton-Raphson is a great iterative solver with one drawback, it is highly sensitive to the initial guess, i.e., the guess has to be sufficiently close to the true solution. The initial guesses used for this program were used after few trial and error applications.
    - The differential equations were further approximated and it was observed that all the quantities can be directly related to Temperature.

- o "Inbuilt"
  - ▪ An inbuilt function "fsolve" from scipy library present in Python was implemented in this program.
  - ▪ "fsolve" is a vector valued solver, i.e., it takes a vector of arguments and gives a vector valued output, thus, it should be handled properly.
  - ▪ "fsolve" takes a transcendental equation as its input and gives out the solution as a vector containing the individual solutions.
  - ▪ This method is not as accurate as the "Self-Coded" program as there is difficulty in defining the stopping criteria. "fsolve" function keeps giving the solutions, even though they are repeated, and thus provides redundant solutions.
  - ▪ Although it is not as good as "Self-Coded" program, but it still gives quite close results. According to this program, blow off occurs at 0.4156 kg/s as opposed to the true value of 0.4150 kg/s.
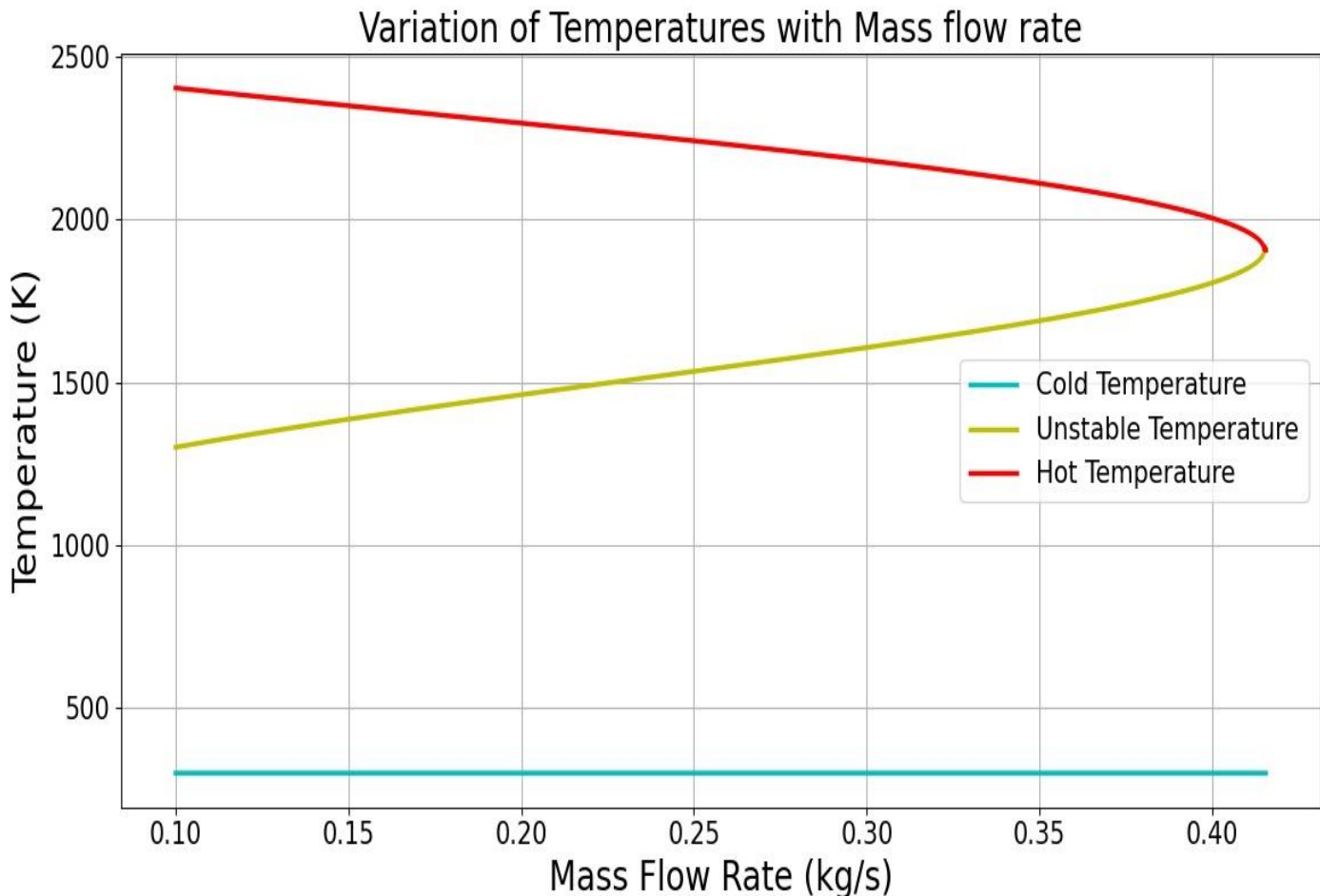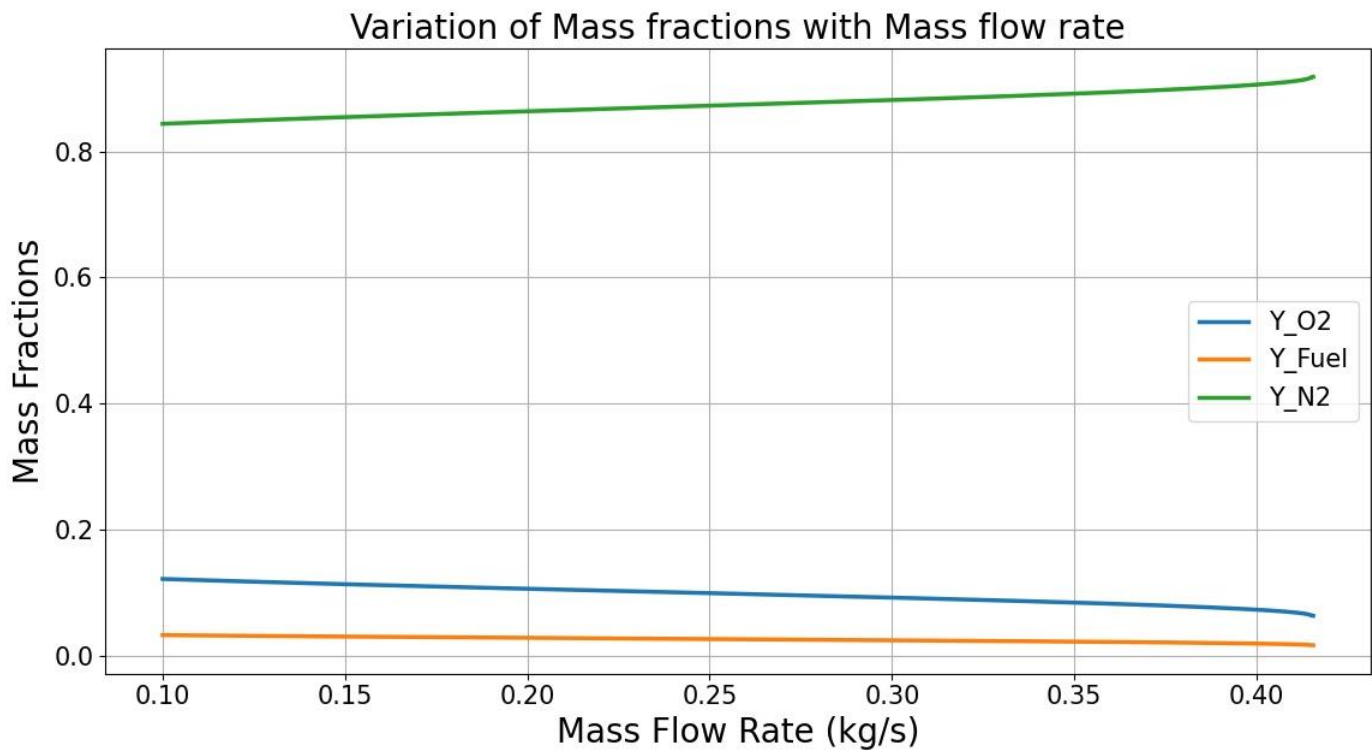 - ▪ The graphs relating to this program are:

Figure 5

Figure 6

CONCLUSIONS/COMMENTS:

- Blow off limit reached for mass flow rate = 0.4151 kg/s
- Final fuel mass fraction: 0.01779
- Final oxygen mass fraction: 0.06469
- Final nitrogen mass fraction: 0.91752
- Final cold temperature: 298.0 K
- Final unstable temperature: 1902.8392 K
- Final hot temperature: 1909.608 K
- The performance of "Self-Coded" program can be increased by using **Intermediate Value Theorem** to shorten the domain sufficiently and then using Newton-Raphson to find the solution.
- An animation showing how the solutions to temperature equations change can be seen using "**Desmos**". Link to the graph is: <u>Animated Graph</u>
- By clicking the "play" button near m variable, the changing values can be seen.
- The solution as obtained from Desmos is $\dot{m} = 0.41160803947777 \, kg/s$ which can not be calculated from the programs as the programs are restricted by the machine limit of my laptop.

Answer 3

The following quantities are given:

1. Ethane (C_2H_6)
2. $Air/Fuel = 16.0$
3. Bore $= 75$ mm
4. Stroke $= 75$ mm
5. $T_i = 300$ K
6. $V_i = 3.68 \times 10^{-4}$ m^3
7. Compression Ratio $= 10:1$
8. $P_i = 1$ atm
9. $\Delta H_f = 4 \times 10^7$ J/kg
10. $C_p = 0.1200 \times 10^4$ J/kg-K
11. $A_f^\star = 6.19 \times 10^9$
12. $x = 0.1$
13. $y = 1.65$
14. $E_T = 15098$
15. $m = 2$
16. $n = 6$
17. $a_{stoic} = m + n/4$

Assumptions made:

i.   One-step global kinetics
ii. The fuel, air, and products all have equal molecular weights; i.e.,

$$M_F = M_{Ox} = M_{Pr} = 29$$

iii. The specific heats of the fuel, air, and products are constants and equal.

$$C_p = 1200 \text{ J / kg-K.}$$

iv. We assume that the stoichiometric air–fuel ratio is 16.0 and restrict combustion to stoichiometric or lean conditions.

The governing equations for the constant volume reactor model are:

From conservation of energy,

$$\dot{Q} - \dot{W} = m\frac{du}{dt}$$

as the work is zero,

$$\frac{\dot{Q}}{m} = \frac{dh}{dt}$$

The system internal energy can be expressed in terms of the system chemical composition:

$$u = \frac{U}{m} = \frac{\sum_{i=1}^{N} N_i \bar{u}_i}{m}$$

Differentiating the above equation gives,

$$\frac{du}{dt} = \frac{1}{m}\left[\sum_i \left(\bar{u}_i \frac{dN_i}{dt}\right) + \sum_i \left(N_i \frac{d\bar{u}_i}{dt}\right)\right]$$

From ideal gas law, we assume that $\bar{u}_i$ is only a function of temperature, i.e., $\bar{u}_i = \bar{u}_i(T)$:

$$\frac{d\bar{u}_i}{dt} = \frac{\partial\bar{u}_i}{\partial T}\frac{dT}{dt} = \bar{C}_{v,i}\frac{dT}{dt}$$

Now,

$$N_i = V[X_i]$$

which upon differentiating gives:

$$\frac{dN_i}{dt} = V\dot{\omega}_i$$

Thus,

$$\frac{du}{dt} = \frac{1}{m}\left[\sum_i (\bar{u}_i V\dot{\omega}_i) + \sum_i \left(N_i \bar{C}_{v,i}\frac{dT}{dt}\right)\right]$$

That leads to the heat equation:

$$\frac{\dot{Q}}{m} = \frac{du}{dt} = \frac{1}{m}\left[\sum_i (\bar{u}_i V\dot{\omega}_i) + \sum_i \left(N_i \bar{C}_{v,i}\frac{dT}{dt}\right)\right]$$

Thus, our energy conservation equation becomes:

$$\frac{dT}{dt} = \frac{(\dot{Q}/V) - \sum_i (\bar{u}_i \dot{\omega}_i)}{\sum_i ([X_i]\bar{C}_{v,i})}$$

for an ideal gas, $\bar{u}_i = \bar{h}_i - R_u T$ and $\bar{C}_{v,i} = \bar{C}_{p,i} - R_u$,

$$\frac{dT}{dt} = \frac{(\dot{Q}/V) + R_u T \sum_i \dot{\omega}_i - \sum_i (\bar{h}_i \dot{\omega}_i)}{\sum_i \left[[X_i](\bar{C}_{p,i} - R_u) \right]}$$

Since we have a constant-volume explosion setup, the rate of change of the pressure is of interest. To calculate dP/dt, we differentiate the ideal-gas law, subject to the constant volume constraint, i.e.,

$$PV = \sum_i N_i R_u T$$

$$V \frac{dP}{dt} = R_u T \frac{d \sum N_i}{dt} + R_u \sum_i N_i \frac{dT}{dt}$$

Applying the definitions of $[X_i]$ and $\dot{\omega}_i$,

$$P = \sum_i [X_i] R_u T$$

Thus, we get the equation for change in pressure with time,

$$\frac{dP}{dt} = R_u T \sum_i \dot{\omega}_i + R_u \sum_i [X_i] \frac{dT}{dt}$$

It is given that the concentration of the fuel is governed by the following equation:

$$\frac{d[F]}{dt} = -A_f^{\star} e^{\left(\frac{-15098}{T}\right)} [F]^x [O_2]^y$$

where we assume that 21% of air is comprised of O_2,

$$[O_2] = 0.21[Ox]$$

Now, relating the oxidizer and product reaction rates to the fuel reaction rate using the stoichiometry,

$$\frac{d[Ox]}{dt} = (A/F)_s \frac{M_F}{M_{Ox}} \frac{d[F]}{dt} = 16 \frac{d[F]}{dt}$$

$$\frac{d[Pr]}{dt} = -[(A/F)_s + 1] \frac{M_F}{M_{Pr}} \frac{d[F]}{dt} = -17 \frac{d[F]}{dt}$$

Now using the equation for temperature:

$$\frac{dT}{dt} = \frac{(\dot{Q}/V) + R_u T \sum_i \dot{\omega}_i - \sum_i (\bar{h}_i \dot{\omega}_i)}{\sum_i \left[[X_i](\bar{C}_{p,i} - R_u)\right]}$$

The above equation is simplified using the assumptions made earlier,

$$\dot{Q}/V = 0 \text{ (adiabatic)}$$

$$\sum \dot{\omega}_i = 0$$

$$\sum \bar{h}_i \dot{\omega}_i = \dot{\omega}_i \bar{h}^o_{f,F}$$

and,

$$\sum [X_i](\bar{C}_{p,i} - R_u) = (\bar{C}_p - R_u) \sum [X_i] = (\bar{C}_p - R_u) \sum \chi_i \frac{P}{R_u T} = (\bar{C}_p - R_u) \frac{P}{R_u T}$$

$$\frac{dT}{dt} = \frac{-\dot{\omega}_F \bar{h}^o_{f,F}}{(\bar{C}_p - R_u)P/(R_u T)}.$$

Now to calculate the rate of change of pressure,

$$P = R_u T([F] + [Ox] + [Pr])$$

or

$$P = P_0 \frac{T}{T_0}$$

differentiating with respect to time,

$$\frac{dP}{dt} = \frac{P}{T}\frac{dT}{dt} = \frac{P_0}{T_0}\frac{dT}{dt}$$

For the initial conditions:

Assuming isentropic compression from bottom-dead-center to top-dead-center and γ, specific heat ratio of 1.4,

The compression ratio is defined as:

$$\text{Compression Ratio} = \frac{V_{\text{BDC}}}{V_{\text{TDC}}}$$

where V_{BDC} and V_{TDS} are the volumes corresponding to the bottom and top dead centers.

The temperature at the top dead center is calculated as follows:

$$T_0 = T_{TDC} = T_{BDC} \left(\frac{V_{BDC}}{V_{TDC}}\right)^{\gamma-1} = 300 \left(\frac{10}{1}\right)^{1.4-1} = 753 \, K$$

and the pressure at the top dead center is calculated as follows:

$$P_0 = P_{TDC} = P_{BDC} \left(\frac{V_{BDC}}{V_{TDC}}\right)^{\gamma} = (1) \left(\frac{10}{1}\right)^{1.4} = 25.12 \, atm$$

$$[Ox]_0 = \left[\frac{(A/F)_s/\Phi}{[(A/F)_s/\Phi] + 1}\right] \frac{P_0}{R_u T_0}$$

$$[F]_0 = \left[1 - \frac{(A/F)_s/\Phi}{[(A/F)_s/\Phi] + 1}\right] \frac{P_0}{R_u T_0}$$

$$[Pr]_0 = 0$$

The above system of equations is solved to obtain the following quantities:

1. Variation of fuel concentration with time
2. Variation of oxygen concentration with time
3. Variation of product concentration with time
4. Variation of temperature with time
5. Variation of pressure with time
6. Variation of rate of change of pressure with time

RESULTS:

The following graphs shows the variation of:

- Fuel concentration
- Oxidizer concentration
- Product concentration
- Temperature
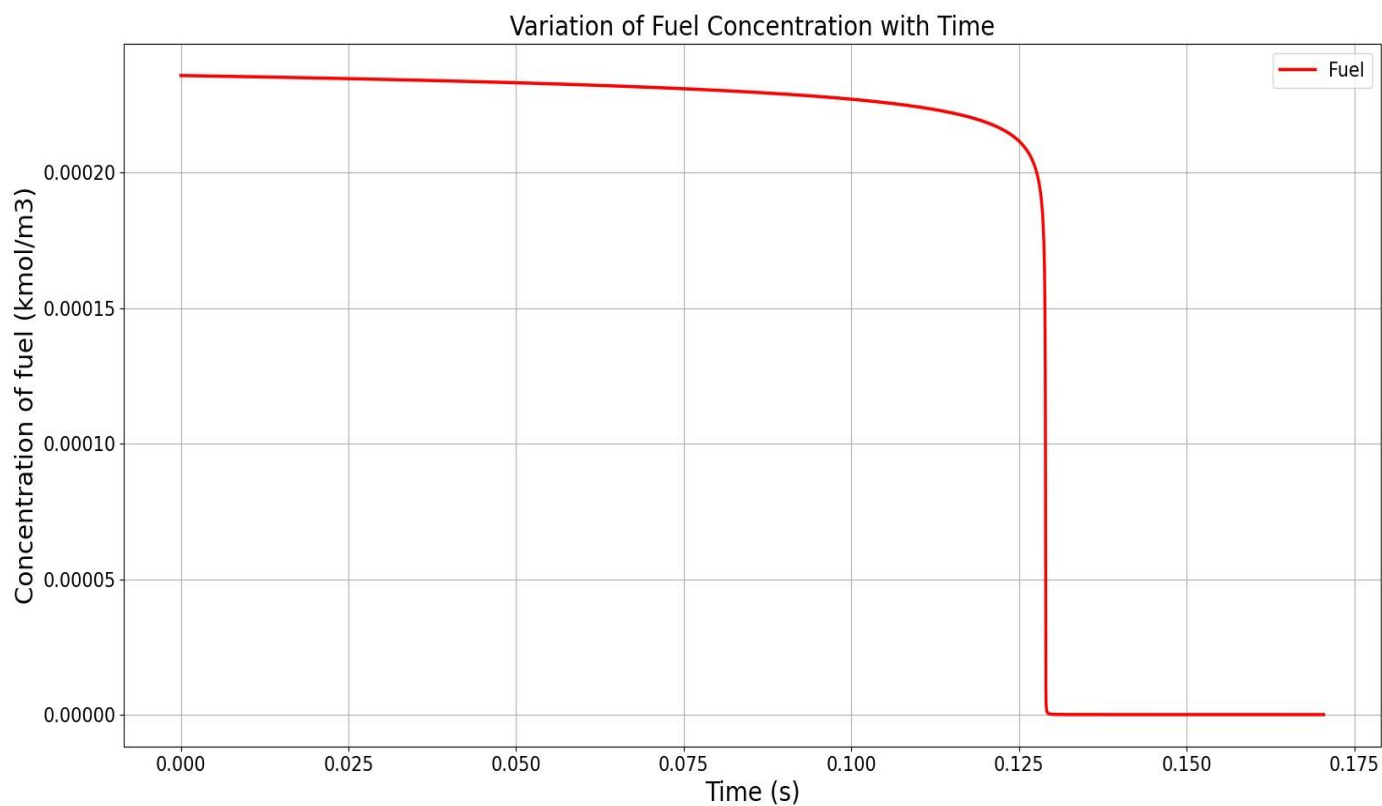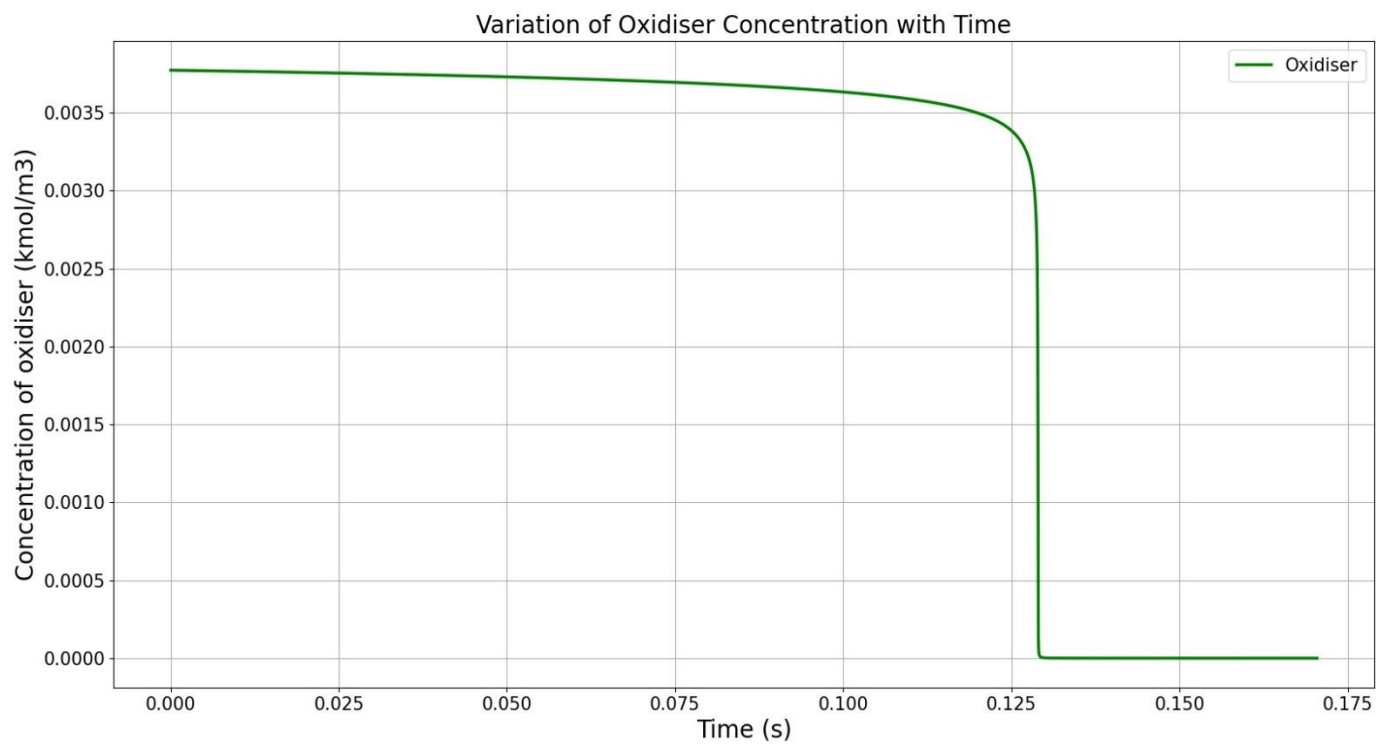- Pressure
- Rate of change of pressure with time
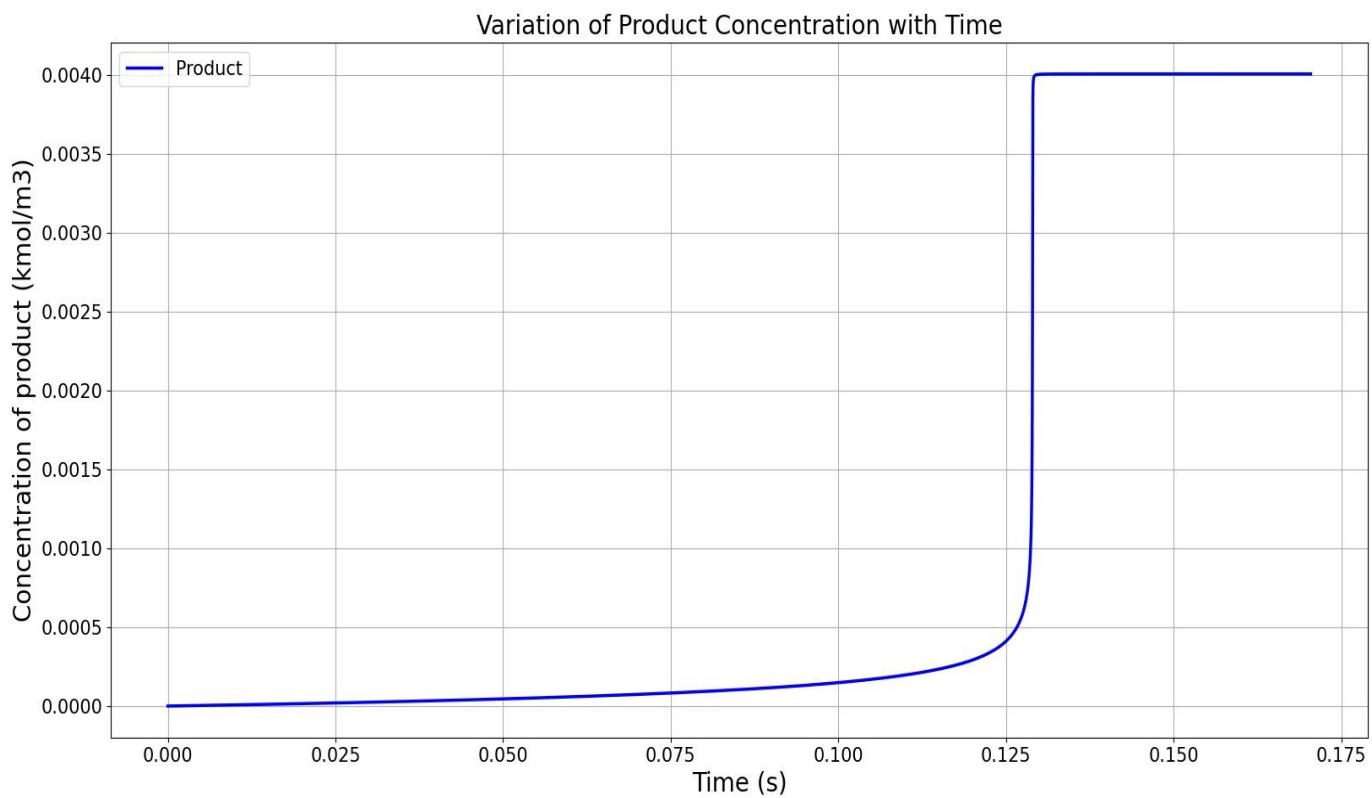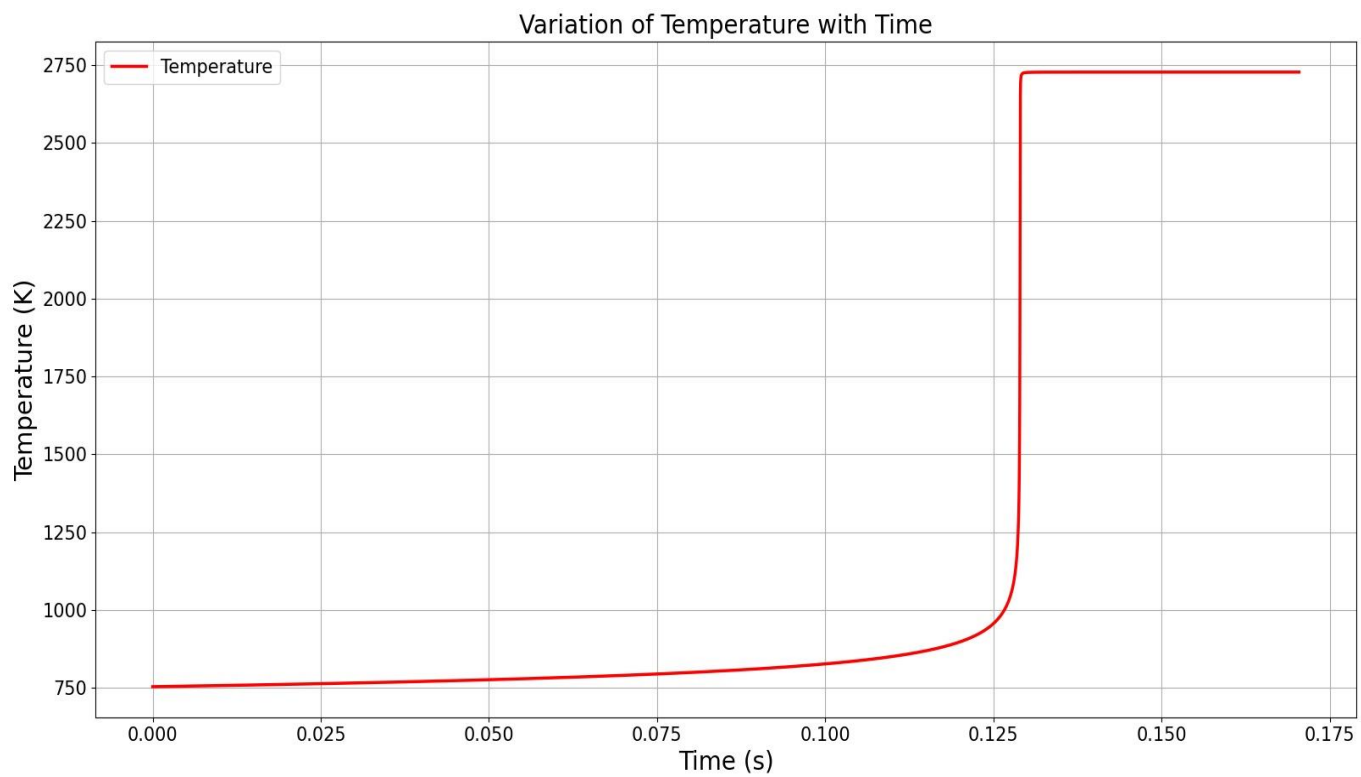
Figure 1

Figure 2

Figure 3

Figure 4

Variation of Pressure with Time
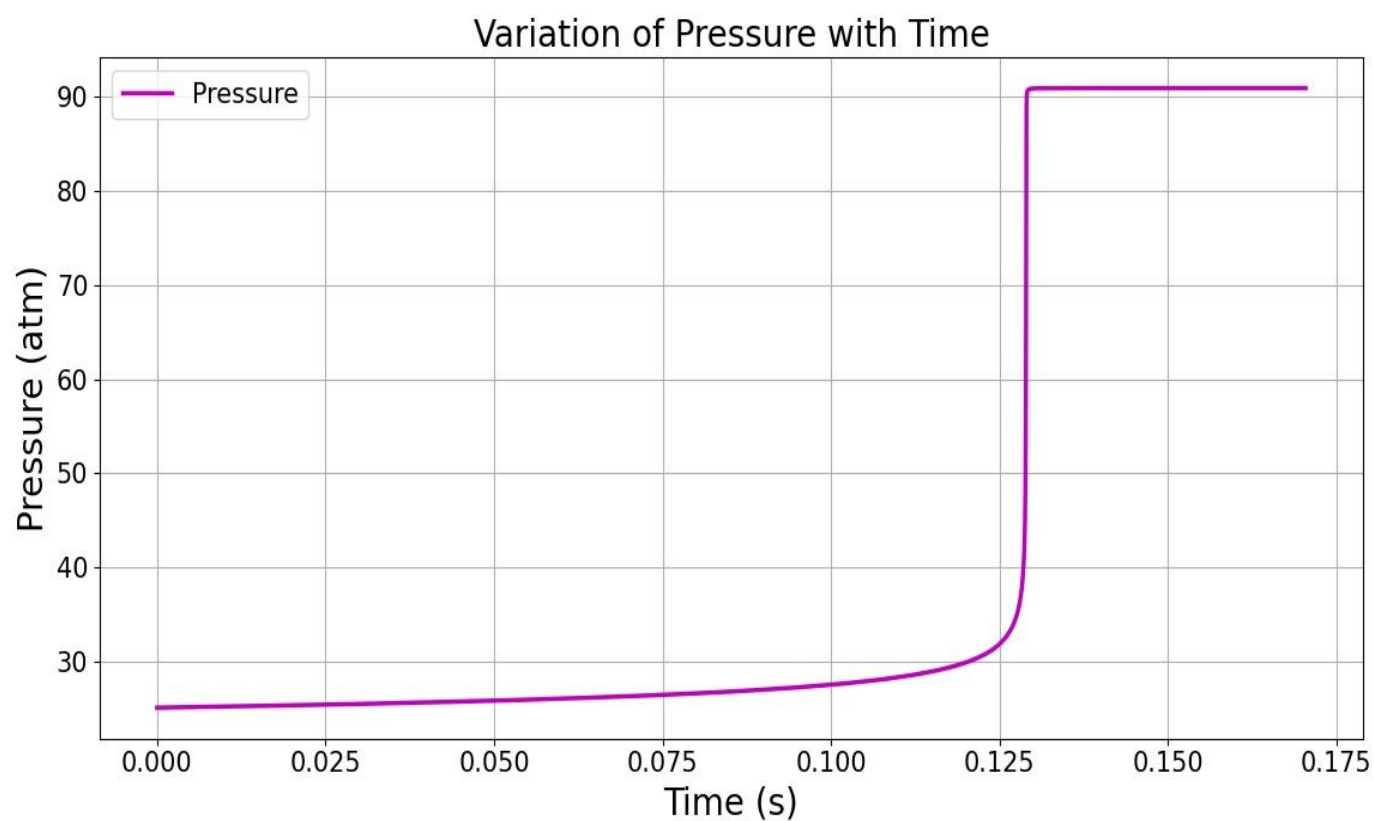

Figure 5
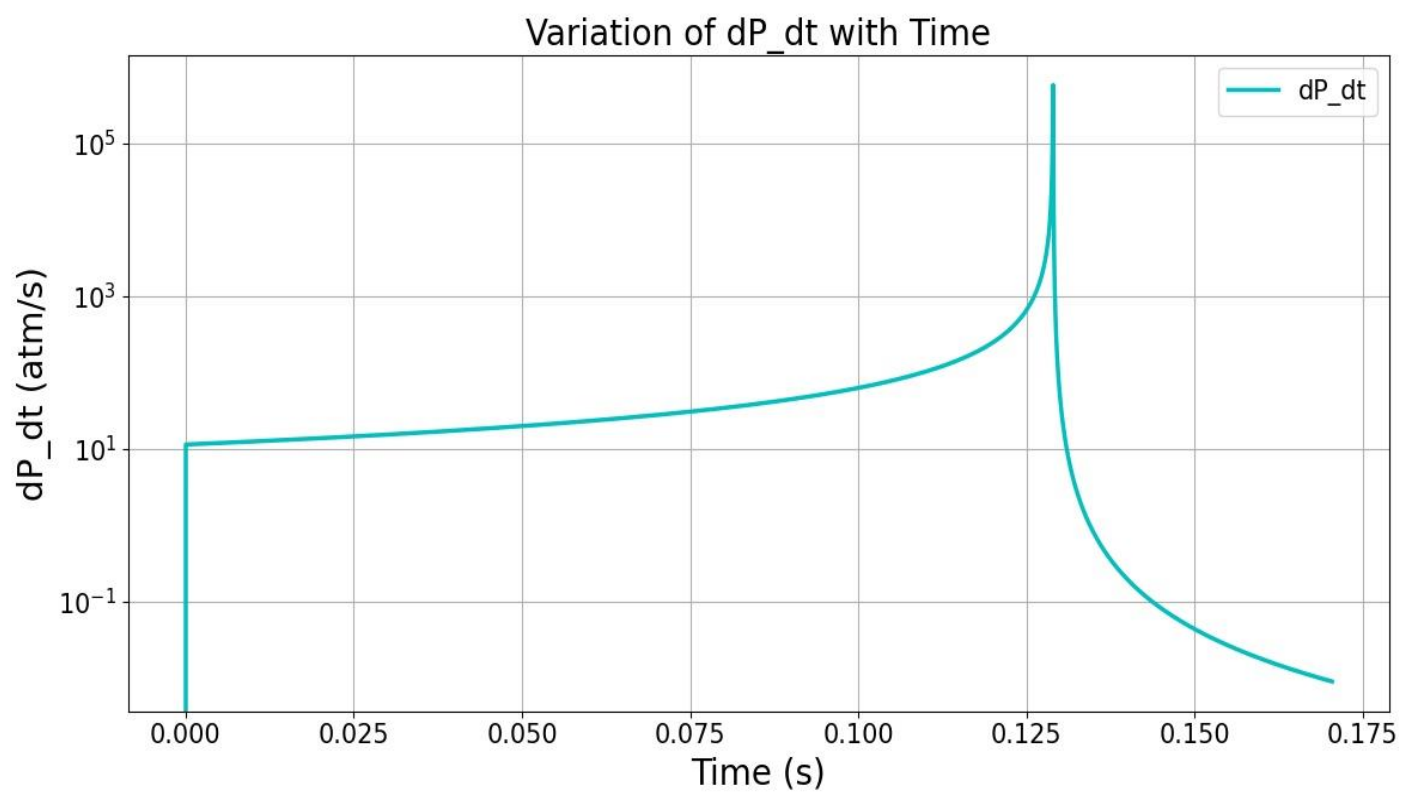
Variation of dP_dt with Time

Figure 6

INTERPRETATIONS:

- The time scale of the entire process is very small, around 175 milliseconds.
- The temperature increases only about 200 K in the first 140 milliseconds, while after that it rises till 2700 K in less than 1 milliseconds, almost instantly.
- The rapid temperature rises and rapid consumption of the fuel is characteristic of a thermal explosion, where the energy released and the temperature rise from reaction feeds back to produce ever-increasing reaction rates because of the $\left[-\dfrac{E_a}{R_u T}\right]$ temperature dependence of the reaction rate.
- Fuel and oxidizer concentration decrease with time as they are being consumed.
- Product concentration, temperature and pressure increase with time.
- For all the above quantities, we see there is a slow change until 175 milliseconds, after which there is almost instant change, with the curve having a slope of almost infinity. This is due to the thermal explosion taking place inside the reactor.
- There is a huge pressure derivative in the explosive stage, with a peak value of about 1.9×10^5 Pa/s.
- This again can be explained using the thermal explosion taking place inside the reactor.
- We have developed two separate programs:
  - "Self-Coded"
    - The differential equations were approximated and it was observed that all the quantities can be directly related to the change in the concentration of the fuel with time.
    - An iterative approach was used and the iterations were carries out until the error was below 10^{-10}.
  - "Inbuilt"
    - An inbuilt function "odeint" from Scipy library present in Python was implemented in this program.
    - "odeint" is a vector valued solver, i.e., it takes a vector of arguments and gives a vector valued output, thus, it should be handled properly.
    - "odeint" takes a system of coupled first order, linear, ordinary, differential equations as its input and gives out the solution as a vector containing the individual solution corresponding to each differential equation.
    - This method provides similar results as of "Self-Coded" program.
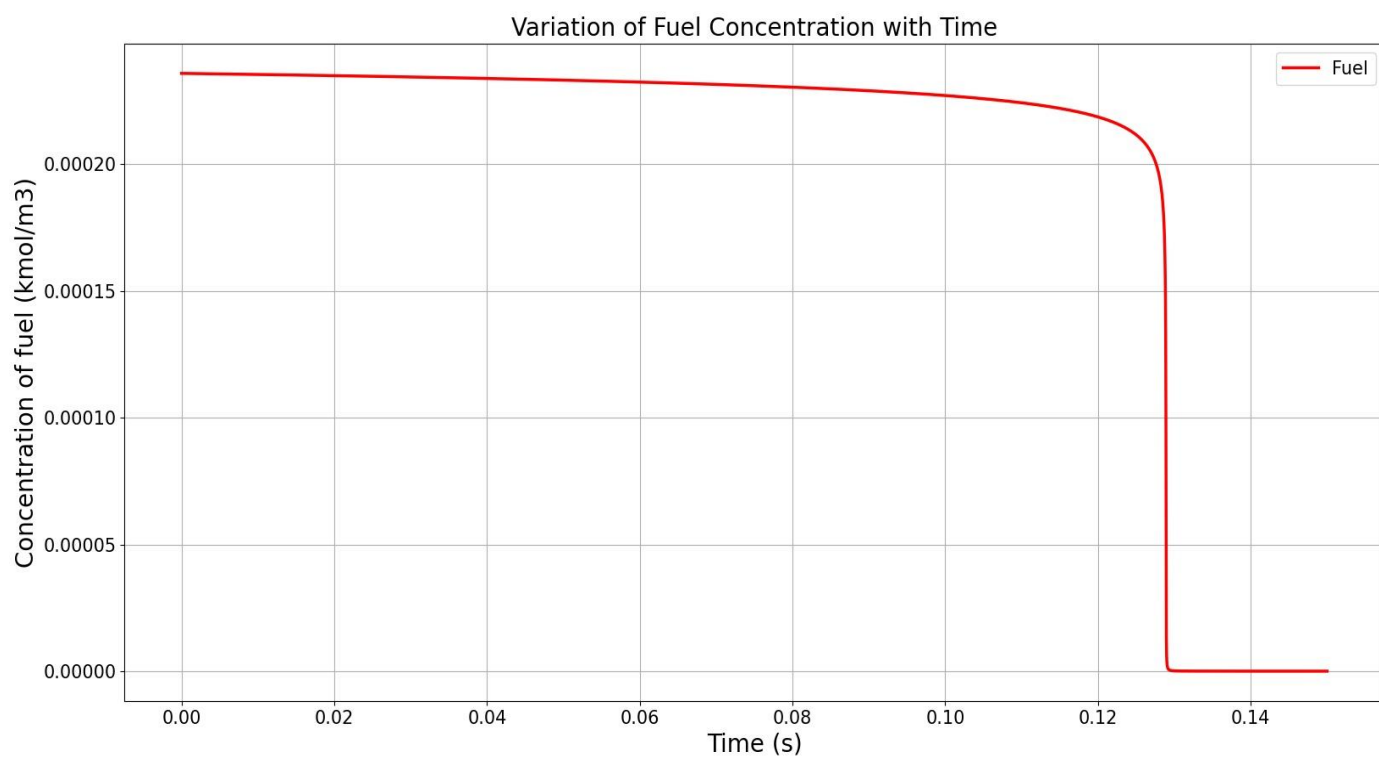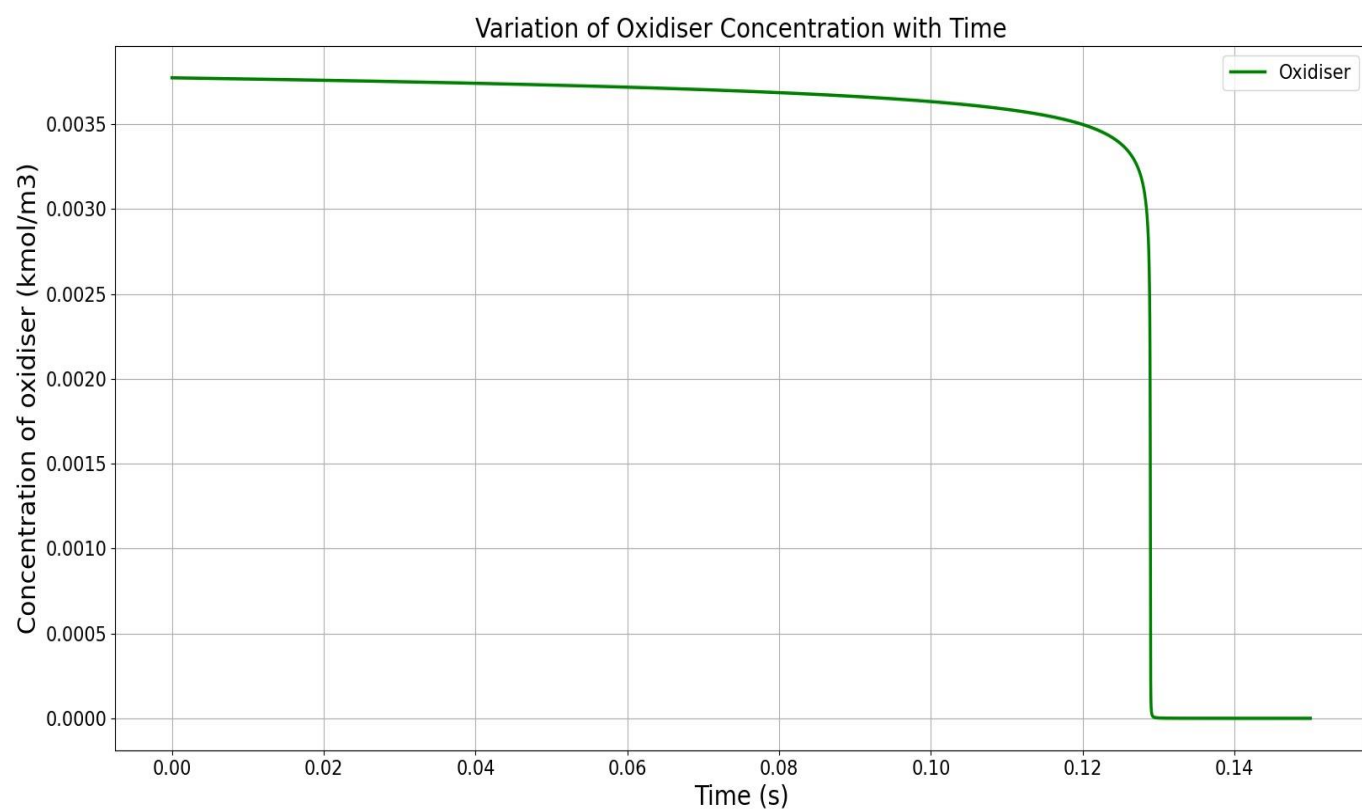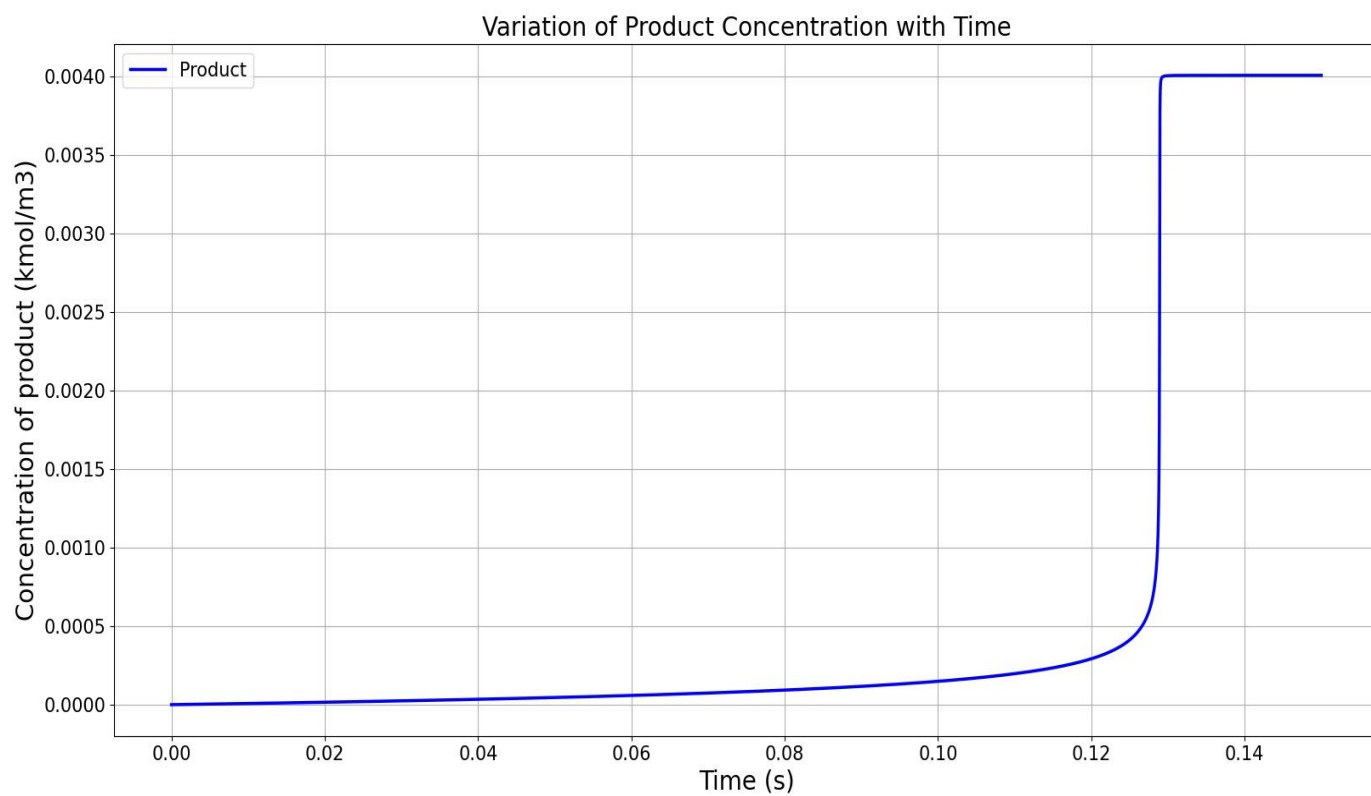   - The graphs relating to this program are shown below:

Figure 7

Figure 8

Variation of Product Concentration with Time

Figure 9
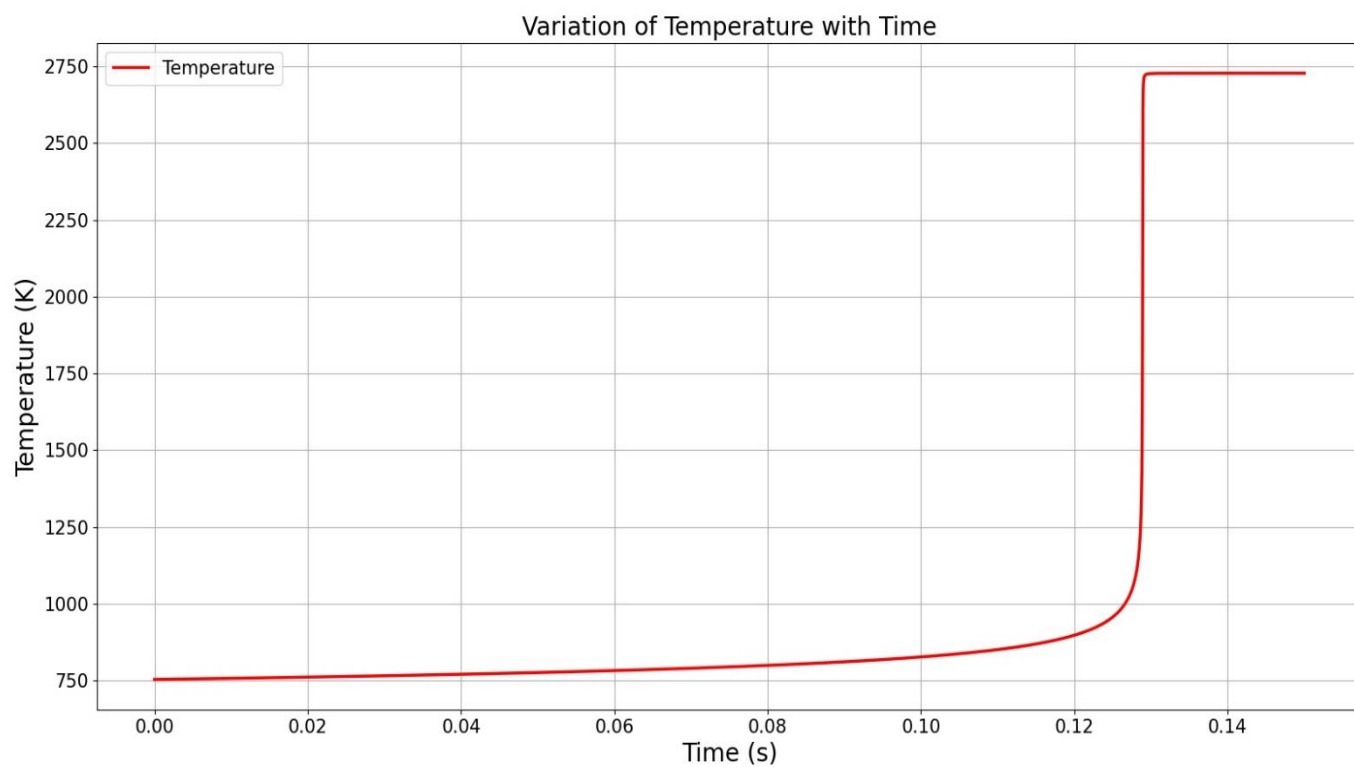

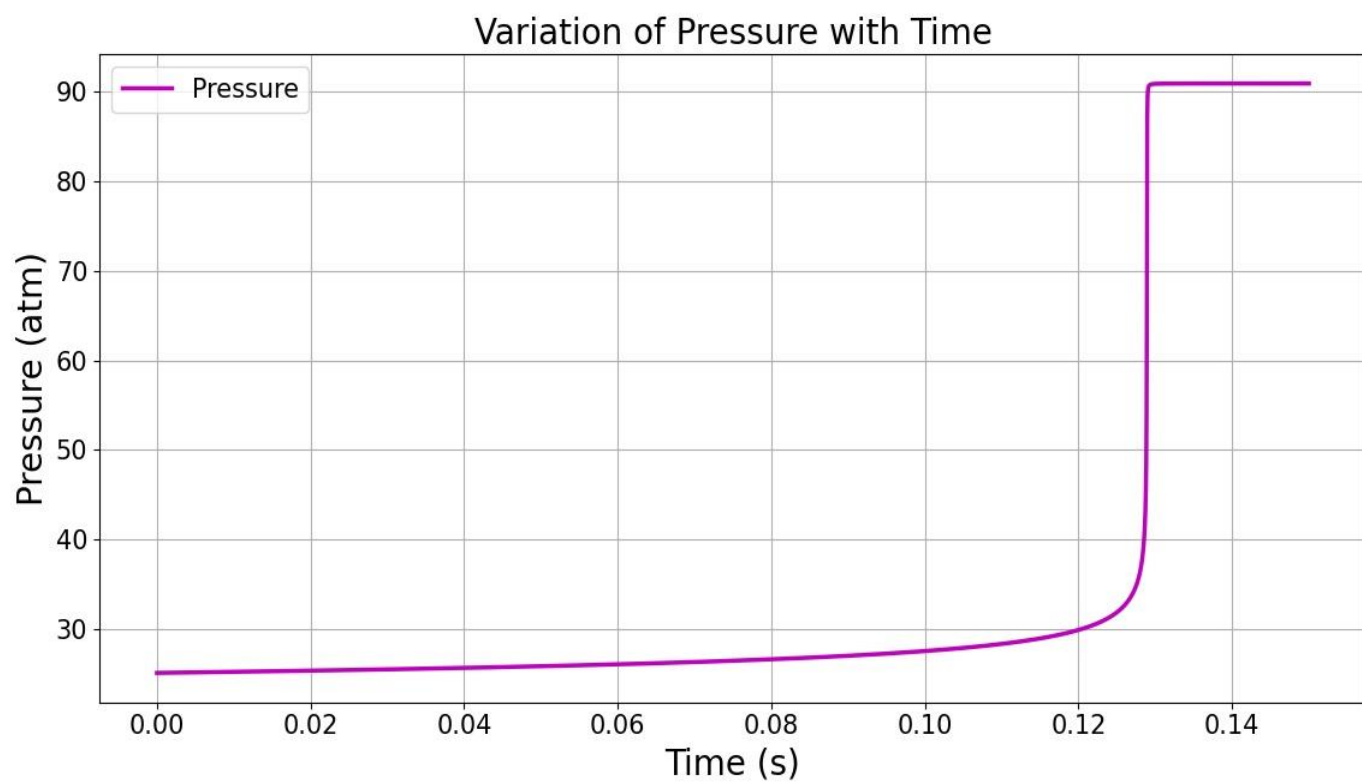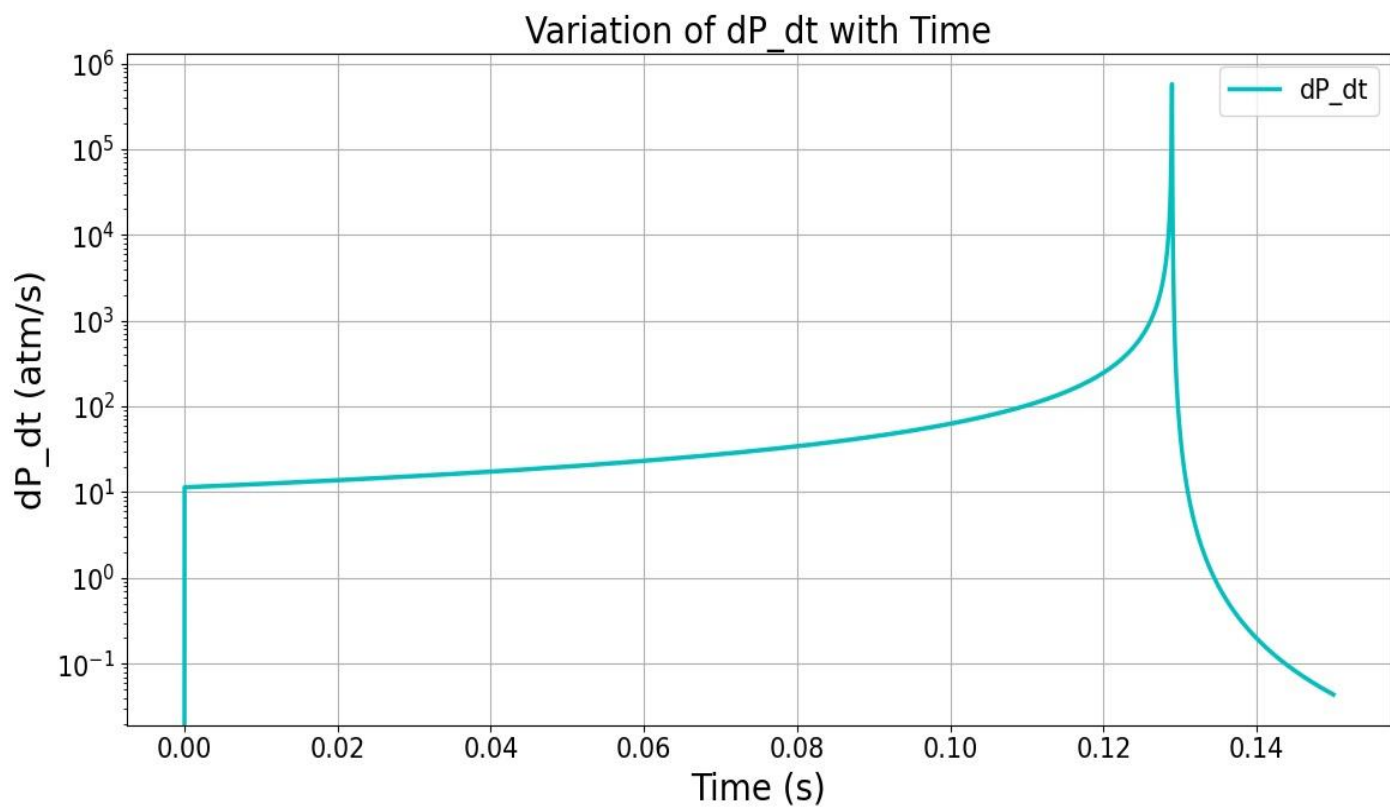## Variation of Temperature with Time

Figure 10

Figure 11

Figure 12

CONCLUSIONS/COMMENTS:

- Although this model predicted the explosive combustion of the mixture after an initial period of slow combustion, as it is observed in real knocking combustion, the single-step kinetics mechanism does not model the true behavior of autoigniting mixtures. In reality, the induction period, or ignition delay, is controlled by the formation of intermediate species, which subsequently react which is only depicted if we use a detailed mechanism.
- There are some problems with the units of quantities mentioned in the question, as they are not clear, so the answer can differ from actual answer by orders of magnitudes, which is only caused by the units.
- All the quantities were plotted and their variation with time was observed.

INDIVIDUAL CONTRIBUTION:

In order to complete the project, we, I and Pranav Aditya Bhatt took the following steps:

1. Understanding the theory behind problems given, deriving the equations and noting down the units for all the quantities.
2. Discussing and understanding the problem and the objectives.
3. Charting out the possible steps that must be taken to solve the problem.
4. Writing the pseudocode for the problem, defining the functions, variables and constants on paper.
5. Writing the actual code with all the functions and plotting relevant results.
6. Discussing the obtained results, and checking whether the solutions made sense or not.
7. If solutions do not make sense, or seem to be wrong, checking back the theory and performing debugging sessions to find any problem in understanding of the problem or the code.
8. Once the correct solution is obtained, comparing them with each other and then writing them out in the report individually.

My contribution in the project were:

1. The code for each problem was prepared individually by both of us. Though the overall structure of the code is similar, we have used different languages, and I have tried to make the code look cleaner and easier to comprehend by:
   a. Defining appropriate functions to perform repetitive task
   b. Writing comments for all parts of code, describing their purpose and functioning
   c. Grouping similar components together for better code readability
   d. Defining proper variable and containers that are self-explanatory of their purpose
2. Using visualization tools like Desmos to get an overview of the problem and its solution. Providing dynamic graphs to see the variation of a quantity that depends on various other parameters.
3. Solving the problems using inbuilt functions and self-written codes.