

Project -2 Report



ME 606 Combustion (Summer 2020)

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Problem 1 A

Problem description

Develop and implement a constant-pressure adiabatic reactor model of combustion of stoichiometric ethane-air mixture. For simplicity, you can assume that the fuel, air, and products have equal molecular weight of 29 and equal specific heat of 1200 J/kg-K. The enthalpy of formation of air and products can be taken to be zero and the enthalpy of formation of the fuel is $4 \times 10^7 \text{ J/kg}$. In addition, one-step global reaction kinetics can be assumed and the fuel reaction rate is:

$$\frac{d[F]}{dt} = -6.19 \times 10^9 \times e^{-\frac{15098}{T}} [F]^{0.1} [O_2]^{1.65} \text{ kmol/m}^3 - s$$

Using an initial volume of 0.008 m^3 , explore the effects of P and T_o on combustion duration.

Equations

Equations for constant pressure reactor

The equations for constant pressure reactor as follows :

$$\frac{d[X_i]}{dt} = \dot{\omega}_i - [X_i] \left[\frac{\sum_i \dot{\omega}_i}{\sum_j [X_j]} + \frac{1}{T} \frac{dT}{dt} \right] \quad 1.1$$

$$\frac{dT}{dt} = \frac{(\dot{Q}/V) - \sum \bar{h}_i \dot{\omega}_i}{\sum [X_i] \bar{c}_{p,i}} \quad 1.2$$

Where $\dot{\omega}_i$ = production rate of i^{th} species ($\text{kmol/m}^3 \text{ s}$)

X_i = concentration of i^{th} species (kmol/m^3)

$\bar{c}_{p,i}$ = constant pressure molar specific heat of i^{th} species ($\text{J/kg} - \text{kmol}$)

\bar{h}_i = molar enthalpy of i^{th} species (J/kmol)

T = Temperature of reactor at time t (K)

Since, the reactor is at constant pressure, volume can change with time. The rate of volume change can be derived from ideal gas equation of state. According to ideal gas equation :

$$PV = \sum_i N_i R_u T$$

Where R_u = Universal Gas constant. On differentiating and dividing by P on both the sides, the equation becomes :

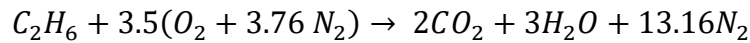
$$\frac{1}{V} \frac{dV}{dt} = \frac{1}{\sum N_i} \sum \frac{dN_i}{dt} + \frac{1}{T} \frac{dT}{dt}$$

Now $\dot{\omega}_i = \frac{1}{V} \frac{dN_i}{dt}$, the equation becomes

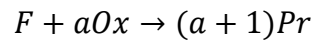
$$\frac{1}{V} \frac{dV}{dt} = \frac{1}{\sum N_i} \frac{\sum \dot{\omega}_i}{V} + \frac{1}{T} \frac{dT}{dt} \quad 1.3$$

Chemical Reaction

The stoichiometric combustion reaction of ethane is



Let us denote ethane (C_2H_6), the fuel for the combustion reaction, by F ; and air, the oxidizer for the combustion by Ox . Products have been denoted by symbol Pr . Let us assume that 1 kg of fuel reacts with a kg of oxidizer to form $(a + 1)$ kg of products. This can be represented by the following reaction.



where $a = \text{Air-fuel ratio at stoichiometry } (A/F)_s = \frac{\text{mass of air}}{\text{mass of fuel}} = \frac{3.5(32+3.76 \times 28)}{30} = 16$

Since the reaction occurs in stoichiometric manner, the mass of fuel and oxidizer consumed in unit time will in the stoichiometric air-fuel ratio.

$$\therefore \frac{\text{mass of oxidizer consumed in unit time}}{\text{mass of fuel consumed in unit time}} = \frac{M_{Ox} \frac{d[Ox]}{dt}}{M_F \frac{d[F]}{dt}} = \left(\frac{A}{F}\right)_s$$

As $M_{Ox} = M_F$

$$\therefore \frac{d[Ox]}{dt} = \left(\frac{A}{F}\right)_s \frac{d[F]}{dt}$$

$$\therefore \frac{d[Ox]}{dt} = 16 \frac{d[F]}{dt}$$

Now

$$\frac{\text{mass of oxidizer} + \text{mass of fuel}}{\text{mass of fuel}} = \frac{A+F}{F}$$

$$\therefore \frac{\text{mass of product formed in unit time}}{\text{mass of fuel consumed in unit time}} = \left(\frac{A+F}{F} \right)$$

$$\therefore \frac{MW_{pr} \frac{d[Pr]}{dt}}{MW_F \left(-\frac{d[F]}{dt} \right)} = \left(\frac{A}{F} + 1 \right)$$

Negative sign because the concentration of fuel is decreasing. As $MW_{pr} = MW_F$, we have the production rate of fuel as

$$\therefore \frac{d[Pr]}{dt} = -(17) \frac{d[F]}{dt}$$

Let us now simplify each of the summation terms appearing in equation (1.1), (1.2) and (1.3)

$$\sum_i \dot{\omega}_i = \dot{\omega}_F + \dot{\omega}_{Ox} + \dot{\omega}_{Pr}$$

$$\sum_i \dot{\omega}_i = \frac{d[F]}{dt} + \frac{d[Ox]}{dt} + \frac{d[Pr]}{dt}$$

$$\sum_i \dot{\omega}_i = \frac{d[F]}{dt} + 16 \frac{d[F]}{dt} - 17 \frac{d[F]}{dt} = 0$$

$$\therefore \sum_i \dot{\omega}_i = 0$$

Now let us simplify $\sum \bar{h}_i \dot{\omega}_i$, where \bar{h}_i is molar enthalpy of i^{th} species. Formation enthalpy of product and oxidizer is zero.

Moreover, all species have equal specific heats, so $\bar{c}_{p,F} = \bar{c}_{p,Ox} = \bar{c}_{p,Pr} = \bar{c}_p$

$$\begin{aligned} \sum \bar{h}_i \dot{\omega}_i &= \bar{h}_F \dot{\omega}_F + \bar{h}_{Ox} \dot{\omega}_{Ox} + \bar{h}_{Pr} \dot{\omega}_{Pr} \\ &= \left(\bar{h}_{f,F} + \bar{c}_p(\Delta T) \right) \dot{\omega}_F + \left(0 + \bar{c}_p(\Delta T) \right) \dot{\omega}_{Ox} + \left(0 + \bar{c}_p(\Delta T) \right) \dot{\omega}_{Pr} \\ &= \bar{h}_{f,F} \dot{\omega}_F + (\dot{\omega}_F + \dot{\omega}_{Ox} + \dot{\omega}_{Pr}) \bar{c}_p(\Delta T) \\ \therefore \sum \bar{h}_i \dot{\omega}_i &= \bar{h}_{f,F} \dot{\omega}_F \quad \left(\text{As } \sum_i \dot{\omega}_i = 0 \right) \end{aligned}$$

Now, $\sum [X_i] \bar{c}_{p,i} = ([F] + [Ox] + [Pr]) \bar{c}_p$

Since the reactor is adiabatic, there is no heat exchange from the reactor $\therefore \dot{Q} = 0$

After using the above simplification, equations (1.1), (1.2) and (1.3) are as follows

$$\frac{d[X_i]}{dt} = \dot{\omega}_i - \frac{[X_i]}{T} \frac{dT}{dt}$$

$$\frac{dT}{dt} = \frac{\bar{h}_{f,F} \dot{\omega}_F}{\bar{c}_p([F] + [Ox] + [Pr])}$$

Note that $\frac{\bar{h}_{f,F}}{\bar{c}_p} = \frac{h_{f,F}}{c_p}$

$$\therefore \frac{dT}{dt} = \frac{h_{f,F} \dot{\omega}_F}{c_p([F] + [Ox] + [Pr])}$$

$$\frac{dV}{dt} = \frac{V}{T} \frac{dT}{dt}$$

$[O_2]$ can be replaced by $[Ox]$, as $[O_2] = 0.21[Ox]$

$$\frac{dT}{dt} = \frac{2.063 \times 10^{14} \times e^{-\frac{15098}{T}} [F]^{0.1} [Ox]^{1.65} \times 0.21^{1.65}}{([F] + [Ox] + [Pr])}$$

Sets of ODEs

$$\frac{dT}{dt} = \frac{1.571 \times 10^{13} \times e^{-\frac{15098}{T}} [F]^{0.1} [Ox]^{1.65}}{([F] + [Ox] + [Pr])}$$

$$\frac{d[F]}{dt} = -6.19 \times 10^9 \times (0.21)^{1.65} \times e^{-\frac{15098}{T}} [F]^{0.1} [Ox]^{1.65} - \frac{[F]}{T} \frac{dT}{dt}$$

$$\frac{d[Ox]}{dt} = -16 \times 6.19 \times 10^9 \times (0.21)^{1.65} \times e^{-\frac{15098}{T}} [F]^{0.1} [Ox]^{1.65} - \frac{[Ox]}{T} \frac{dT}{dt}$$

$$\frac{d[Pr]}{dt} = 17 \times 6.19 \times 10^9 \times (0.21)^{1.65} \times e^{-\frac{15098}{T}} [F]^{0.1} [Ox]^{1.65} - \frac{[Pr]}{T} \frac{dT}{dt}$$

$$\frac{dV}{dt} = \frac{V}{T} \frac{1.571 \times 10^{13} \times e^{-\frac{15098}{T}} [F]^{0.1} [Ox]^{1.65}}{([F] + [Ox] + [Pr])}$$

These five ODEs are to be solved for initial conditions of $[F]_o, [Ox]_o, [Pr]_o, T_o$ and V_o

Initial conditions

At $t = 0$, the mole-fractions of fuel, oxidizer and product can be calculated as follows:

$$\phi = \frac{F/A}{(F/A)_s} = \frac{N_F MW_F}{N_A MW_A} 16 \quad \text{and} \quad MW_F = MW_A$$

$$\therefore \text{mole of air } N_A = \frac{16N_F}{\phi}$$

$$\chi_{Ox} = \frac{N_A}{N_A + N_F} = \frac{\frac{16}{\phi}}{\frac{16}{\phi} + 1} = 0.94 \quad \text{and} \quad \chi_F = 1 - \chi_{Ox} = 0.06$$

$$\chi_{Pr} = 0, \quad V_o = 0.008 \text{ m}^3$$

$[X_i]$ can be calculated as $[X_i] = \frac{P\chi_i}{R_u T_o}$. So, given T_o and P one can find out initial concentration of species.

Thus there are five initials values ($[F], [Ox], [Pr], T_o, P$) for the five coupled linear ODEs.

Procedure

The five coupled linear ODEs, are solved for some particular value of T_o and P by using the ODE solver of MATLAB. The concentration terms changes very fast in comparison to the temperature. Thus, the set of ODEs are stiff ODEs. A stiff ODE solver of MATLAB like ode15s or ode23s can be used to solve stiff ODEs. We have used ode15s to solve the ODEs for this problem. The code ProbA1.m has been provided in the zip folder.

First of all, the ODEs, were written in the functional file of ODEsA1.m; the constants like formation enthalpy of fuel, specific heat, molecular mass etc. were defined in the functional file itself. The ODEs were solved from the main file of ProbA1.m

To study the effect of P and T_o , ProbA1.m solves the ODEs and determine the combustion time, for a given array of initial temperature and pressure.

Combustion time is defined as the time at which the concentration of fuel decreases by 1000 times the initial concentration. So, for every value T_o and P , a while loop is iterated over all the calculated values of fuel concentration $[F]$, and the index at which the fuel concentration decreases by 1000 times is determined. From the index, the combustion time could be obtain.

Results

Combustion time was determined for four different values of pressure, and five different values of temperature starting from 600 K to 1000 K, increasing the temperature in step of 100. Combustion time is tabulated below

	Pressure P				
Temperature (T_o) (K)	1 atm	2 atm	5 atm	25 atm	
600	3.9991	2.3919	1.2101	0.3627	Combustion time (s)
700	0.1747	0.1044	0.0528	0.0158	
800	0.0180	0.0108	0.0054	0.0016	
900	0.0034	0.002	0.001	3.07E-04	
1000	0.0010	0.0006	0.0003	9.46E-05	

Table 1 Variation of Combustion time(s) on T_o and P

A chart of combustion time versus initial temperature, for different values of pressure has been plotted on logarithmic time scale.

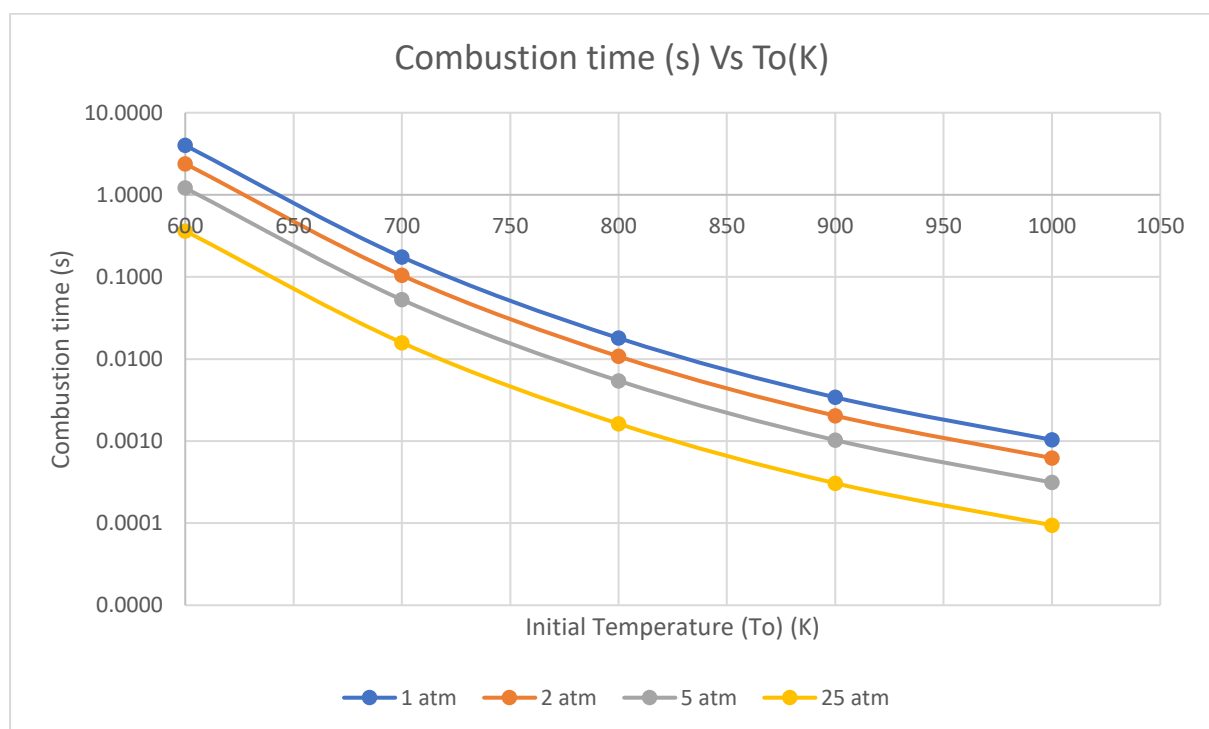


Figure 1 Plot of combustion time vs. initial temperature

A chart of Concentration versus time is shown below :

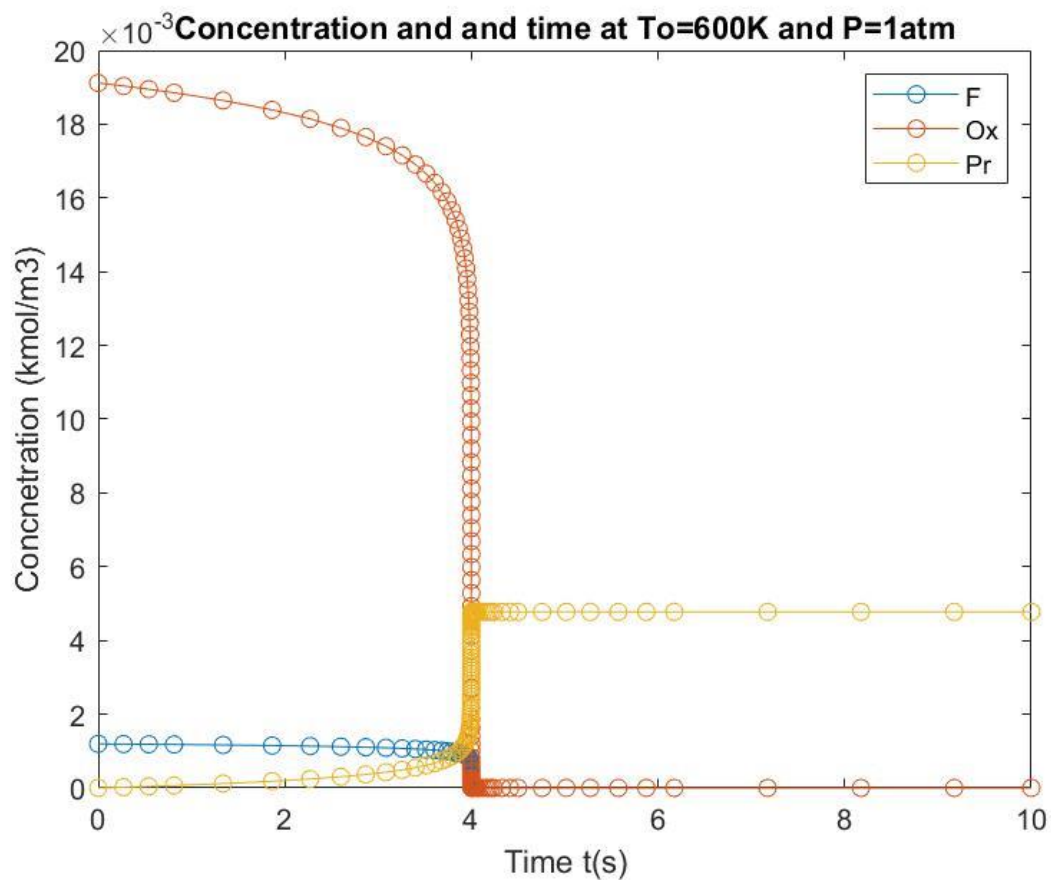


Figure 2 Concentration versus time at $T_o = 600\text{ K}$ and $P = \text{atm}$

Discussion

From the graph above, it is observed that increasing the pressure reduces the time to complete the reaction. Increasing pressure reduces the mean free path of molecule, which increases the probability of molecules colliding with other molecules to form the desired product, hence increasing the rate of reaction, thus decreasing the time for combustion.

It is also observed that increasing the temperature also reduces the time to complete combustion reaction. Increasing the temperature will increase the speed of the molecules which will increase the probability of colliding with other molecules to form the products, hence decreasing the time for complete combustion. By increasing the temperature the kinetic energy of molecules increases, thus the activation energy barrier decreases, which in turn increases the rate of reaction. Thus, ultimately reducing the time for combustion.

Theoretically the reactor should be operated at maximum temperature and pressure, to get reaction done in least time. However, the initial temperature and pressure are bound by other factors like the material of conducting duct, material of reactor, etc. In practice an optimal value of initial temperature and pressure is selected, to complete the reaction in minimum time.

Conclusion

Increasing Pressure and Increasing Temperature will reduce the time for complete combustion. Thus to get products in minimum time, the reactor should be operated with maximum possible initial temperature and pressure.

Problem 2 B

Problem description

Develop a plug-flow-reactor model using the same chemistry and thermodynamics as in problem A1. Assume the reactor is adiabatic. Use the model to

1. Determine the mass flowrate such that the reaction is 99 percent complete in a flow length of 10 cm for $T_{in} = 1000$ K, $P_{in} = 0.2$ atm, and $\phi = 0.2$. The circular duct has a diameter of 3 cm.
2. Explore the effects of P_{in} , T_{in} and ϕ on the flow length required for 99 percent complete combustion using the determined flowrate.

$$\frac{d[F]}{dt} = -6.19 \times 10^9 \times e^{-\frac{15098}{T}} [F]^{0.1} [O_2]^{1.65} \text{ kmol/m}^3 - s$$

Equations

Since, the reactor is adiabatic the heat exchange from reactor is zero, i.e. $\dot{Q} = 0$.

The equations for plug flow reactor as follows :

Mass Equation :

$$\begin{aligned} \frac{d(\rho v_x A)}{dx} &= 0 \\ \therefore \rho \frac{dv_x}{dx} + v_x \frac{d\rho}{dx} &= 0 \end{aligned} \quad (2.1)$$

Species Conservation:

$$\rho v_x \frac{d(Y_i)}{dx} = \dot{\omega}_i MW_i \quad (2.2)$$

Momentum Equation :

$$\rho v_x \frac{d(v_x)}{dx} + \frac{dP}{dx} = 0 \quad (2.3)$$

Energy Conservation :

$$\frac{d(h + v_x^2/2)}{dx} = 0 \quad (2.4)$$

Now as $h = h(T, Y_i)$, using chain Rule to relate dh/dx with dT/dx

$$\frac{dh}{dx} = c_p \frac{dT}{dx} + \sum_i h_i \frac{dY_i}{dx}$$

So, equation-(4) becomes

$$c_p \frac{dT}{dx} + \frac{\sum_i h_i \dot{\omega}_i MW_i}{\rho v_x} + v_x \frac{dv_x}{dx} = 0$$

From equation (2.1), we have $\frac{dv_x}{dx} = -\frac{v_x}{\rho} \frac{d\rho}{dx}$, substituting this in above equation, we get

$$\frac{dT}{dx} = \frac{v_x^2}{\rho} \frac{d\rho}{dx} - \frac{\sum_i h_i \dot{\omega}_i MW_i}{c_p \rho v_x} \quad (2.5)$$

Ideal Gas Law

$$P = \frac{\rho R_u T}{MW_{mix}}$$

On differentiating the ideal gas equation, and dividing by P on both the sides, we get

$$\frac{1}{P} \frac{dP}{dx} = \frac{1}{\rho} \frac{d\rho}{dx} + \frac{1}{T} \frac{dT}{dx}$$

Eliminating the dT/dx and dP/dx terms from the above equation, by using equations (2.3) and (2.4), $d\rho/dx$ is given by

$$\frac{d\rho}{dx} = \frac{\frac{\rho R_u}{v_x c_p MW_{mix}} (\sum_i h_i \dot{\omega}_i MW_i)}{P \left(1 + \frac{v_x^2}{c_p T} \right) - v_x^2 \rho}$$

Where $\dot{\omega}_i$ = production rate of i^{th} species (kmol / m³s)

Y_i = Mass Fraction of i^{th} species (kg/kg)

$c_{p,i}$ = constant pressure specific heat of i^{th} species (J/kg – K)

h_i = enthalpy of i^{th} species (J/kg)

ρ = Density (kg/m³)

P = Pressure of the mixture (Pa)

v_x = velocity in of mixture in x-direction (m/s)

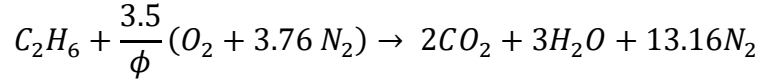
MW_i = Mass of i^{th} species (kg)

A = Cross-sectional area of Plug – flow reactor (m²)

$$T = \text{Temperature of reactor} \quad (K)$$

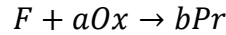
Chemical Reaction

The combustion reaction of ethane for lean condition is



Where $\phi = 0.2$, equivalence ratio

The reaction can be represented in terms of mass of fuel and oxidizer. Let a be the air-fuel ratio for the given value of equivalence ratio.



$$\text{Air-fuel ratio at stoichiometry } (A/F)_s = \frac{\text{mass of air}}{\text{mass of fuel}} = \frac{3.5(32+3.76 \times 28)}{30} = 16$$

$$\text{Air-fuel ratio actual } (A/F)_{actual} = \frac{(A/F)_s}{\phi} = \frac{16}{0.2} = 80$$

$$\text{Now, } \frac{\text{mass of oxidizer consumed in unit time}}{\text{mass of fuel consumed in unit time}} = \frac{M_{Ox} \frac{d[Ox]}{dt}}{M_F \frac{d[F]}{dt}} = \frac{A}{F}$$

$$\text{As } M_{Ox} = M_F$$

$$\therefore \frac{d[Ox]}{dt} = \left(\frac{A}{F}\right) \frac{d[F]}{dt}$$

$$\therefore \frac{d[Ox]}{dt} = 80 \frac{d[F]}{dt}$$

$$\text{Now } \frac{\text{mass of oxidizer} + \text{mass of fuel}}{\text{mass of fuel}} = \frac{A+F}{F}$$

$$\therefore \frac{\text{mass of product formed in unit time}}{\text{mass of fuel consumed in unit time}} = \left(\frac{A+F}{F}\right)$$

$$\therefore \frac{MW_{pr} \frac{d[Pr]}{dt}}{MW_F \left(-\frac{d[F]}{dt}\right)} = \left(\frac{A}{F} + 1\right)$$

Negative sign because the concentration of fuel is decreasing. Also $MW_{pr} = MW_F$, we have the production rate of fuel as

$$\therefore \frac{d[Pr]}{dt} = -(81) \frac{d[F]}{dt}$$

Simplifying $\sum h_i \dot{\omega}_i MW_i$, where \bar{h}_i is molar enthalpy of i^{th} species.

Formation enthalpy of product and oxidizer is zero. Moreover, $\bar{c}_{p,F} = \bar{c}_{p,Ox} = \bar{c}_{p,Pr} = \bar{c}_p$ and all species have same molecular mass.

$$\begin{aligned} \sum h_i \dot{\omega}_i MW_i &= h_F \dot{\omega}_F MW_F + h_{Ox} \dot{\omega}_{Ox} MW_{Ox} + h_{Pr} \dot{\omega}_{Pr} MW_{Pr} \\ &= \left[(h_{f,F} + \bar{c}_p(\Delta T)) \dot{\omega}_F + (0 + \bar{c}_p(\Delta T)) \dot{\omega}_{Ox} + (0 + \bar{c}_p(\Delta T)) \dot{\omega}_{Pr} \right] MW \\ &= [h_{f,F} \dot{\omega}_F + (\dot{\omega}_F + \dot{\omega}_{Ox} + \dot{\omega}_{Pr}) \bar{c}_p(\Delta T)] MW \\ &\therefore \sum h_i \dot{\omega}_i MW_i = h_{f,F} \dot{\omega}_F MW \end{aligned}$$

Conversion of mass fraction to concentration

$$\begin{aligned} X_i &= \frac{\chi_i P}{R_u T} = \frac{Y_i MW_{mix}}{MW_i} \frac{\rho R_u T}{M_{mix}} \frac{1}{R_u T} \\ &\therefore X_i = \frac{Y_i \rho}{MW_i} \end{aligned}$$

Let \dot{m} , be the mass flow-rate. Mass flow rate can be related to velocity and density as follows. Here A , is the cross-sectional area of the circular reactor.

$$\dot{m} = \rho v_x A$$

Sets of ODEs

$$\begin{aligned} \frac{d[X_i]}{dt} &= \frac{\dot{\omega}_i}{v_x} \\ \frac{dT}{dx} &= \frac{v_x^2}{\rho} \frac{d\rho}{dx} - \frac{MW h_{f,F} \dot{\omega}_F}{c_p \rho v_x} \\ \frac{d\rho}{dx} &= \frac{\frac{\rho R_u}{v_x c_p MW_{mix}} (\sum_i h_i \dot{\omega}_i MW_i)}{P \left(1 + \frac{v_x^2}{c_p T} \right) - v_x^2 \rho} \end{aligned}$$

v_x and P can be eliminated from above equations by using mass-flow rate equation and the ideal-gas equation.

$$\dot{m} = v_x \rho A$$

$$P = \frac{\rho R_u T}{MW}$$

So, for a given mass-flow rate one can solve for the concentrations at the end of the reactor.

Initial conditions

At the inlet of the reactor, at $x = 0$, the mole-fractions of fuel, oxidizer and product are calculated as follows :

$$\phi = \frac{F/A}{(F/A)_s} = \frac{N_F MW_F}{N_A MW_A} 16 \quad \therefore \text{mole of air } N_A = \frac{16}{\phi} N_F$$

$$\chi_{Ox} = \frac{N_A}{N_A + N_F} = \frac{(16/\phi)}{(16/\phi) + 1} = 0.988 \quad \text{and} \quad \chi_F = 1 - \chi_{Ox} = 0.012$$

$$\chi_{Pr} = 0,$$

Mass-fraction is related to mole-fraction as $Y_i = \frac{MW_i}{MW_{mix}} \chi_i$. All species have equal molecular mass. So, $Y_i = \chi_i$

$$\therefore Y_F = 0.012 \quad ; \quad Y_{Ox} = 0.988 \quad ; \quad Y_{Pr} = 0$$

$$T_{in} = 1000 \text{ K} \quad \text{and} \quad P_{in} = 0.2 \text{ atm}$$

$$\therefore \rho_{in} = \frac{P_{in} MW_{mix}}{R_u T_{in}} = \frac{0.2 \times 101325 \times 29 \times 10^{-3}}{8.314 \times 1000} = 0.0707 \text{ kg/m}^3$$

Procedure

The set of ODEs consists of eight unknowns ($[F]$, $[Ox]$, $[Pr]$, ρ , T , v_x , P , \dot{m}). There are seven independent equations. The problem requires to determine the mass-flow rate such that the reaction is 99% complete.

To obtain the mass-flow rate, initially a guessed value of mass-flow rate $\dot{m} = 1 \text{ kg/s}$ was selected and the equations were solved for the flow length of 10 cm . If the fuel concentration gets reduced to 1% of the initial concentration, then that mass-flow rate is selected. If the fuel concentration is larger than 1% of initial concentration, then another guess of mass-flow rate is made, and the process is repeated until a correct value of mass-flow rate is not obtained. Mass-flow rate is decreased in steps of 0.0001

The ODEs, were solved using the MATLAB ODE solver, ode45.

```

Editor - C:\Users\dell\Documents\Sem-4\ME 606 Combustion\Project-2\ProbB2.m
25 - YPr = 0;
26 - yo = [XF; XOx; XPr; Tin; Rhoin];
27
28 - massFlow = 0;
29
30 - [x,y] = ode45(@(x,y) ODEsB2(x,y, m_dot), [0,0.1], yo);
31 - while(massFlow == 0)
32 -     m_dot = m_dot - 0.01;
33 -     [x,y] = ode15s(@(x,y) ODEsB2(x,y, m_dot), [0,0.1], yo);
34 -     if (y(length(y(:,1)), 1) <= (0.01*XF))
35 -         massFlow = m_dot;
36 -     end
37 - end
38
39 - velocity = massFlow/A*y(:,5);
40 - disp("The mass-flow rate for 99% reaction is " + massFlow + " kg/m3.");

```

ODEsB2.m x ProbB2.m x +

Command Window

```

>> ProbB2
The mass-flow rate for 99% reaction is 0.26 kg/m3.
fx >>

```

Figure 3 MATLAB code to calculate mass-flow rate for 99% reaction

To study the effect of P_{in} , T_{in} and ϕ on the Flow-length, another program, probB2_2.m was written in MATLAB. The mass-flow rate from pat-1 was used to determine the flow-length needed for 99% reaction.

For every given value of T_{in} , P_{in} and ϕ the ODEs were solved by taking sufficiently large value of flow-length x . After that a loop is iterated over the fuel concentration, and the index at which the concentration is 1% of initial concentration, is determine. By knowing the index, the flow-length could be determined from the array of x .


```

36 -         index = 0;
37 -         count=1;
38 -         while(index==0 && count <= length(x))
39 -             if(y(count,1) <= XF*0.01)
40 -                 index = count;
41 -             end
42 -             count = count + 1;
43 -         end
44 -         %flowLength(i,j,k)=x(index);
45 -         %flowLength(k)=x(index);
46 -         disp("The flow-length is " + x(index) + " m");
47 -     end
48 - end
49 -
ODEsB2_2.m ProbB2_2.m +
Command Window
>> ProbB2_2
The flow-length is 0.24809 m
The flow-length is 0.15135 m
The flow-length is 0.099984 m
The flow-length is 0.031004 m
The flow-length is 0.024311 m
The flow-length is 0.022214 m
The flow-length is 0.021417 m
fx>>

```

Figure 4 MATLAB program to determine flow length, by varying T_{in} , P_{in} and ϕ

Results

The sets of ODEs, were solved in MATLAB ODE solver ode45. The initial guess value of flow rate was 1 kg/s. To get more precise value of mass-flow rate, \dot{m} was reduced in steps of 0.0001.

After running the code ProbB2_1, the value of **mass flow** rate is obtained as **0.2655 kg/s**.

To study the effect of P_{in} , T_{in} and ϕ on the Flow-length, another program was written to calculate flow-length.

The variation on flow-length with P_{in} and T_{in} for different ϕ are as follows

For $\phi = 0.2$

At $\phi = 0.2$, flow-length is tabulated, for given values of P_{in} and T_{in}

At $\phi = 0.2$	Temperature (T_{in}) (K)				
Pressure (P_{in}) (atm)	800 K	900 K	1000 K	1100 K	
0.2	89.81	25.03	10.00	5.04	Flow-Length (cm)
0.5	19.41	5.76	2.33	1.13	
1	4.59	1.12	0.49	0.28	
1.5	2.16	0.43	0.15	0.09	

2	1.29	0.24	0.07	0.04	
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Table 2 Table of flow-length for $\phi = 0.2$

A chart showing the variation of flow length with P_{in} and T_{in} is given below.

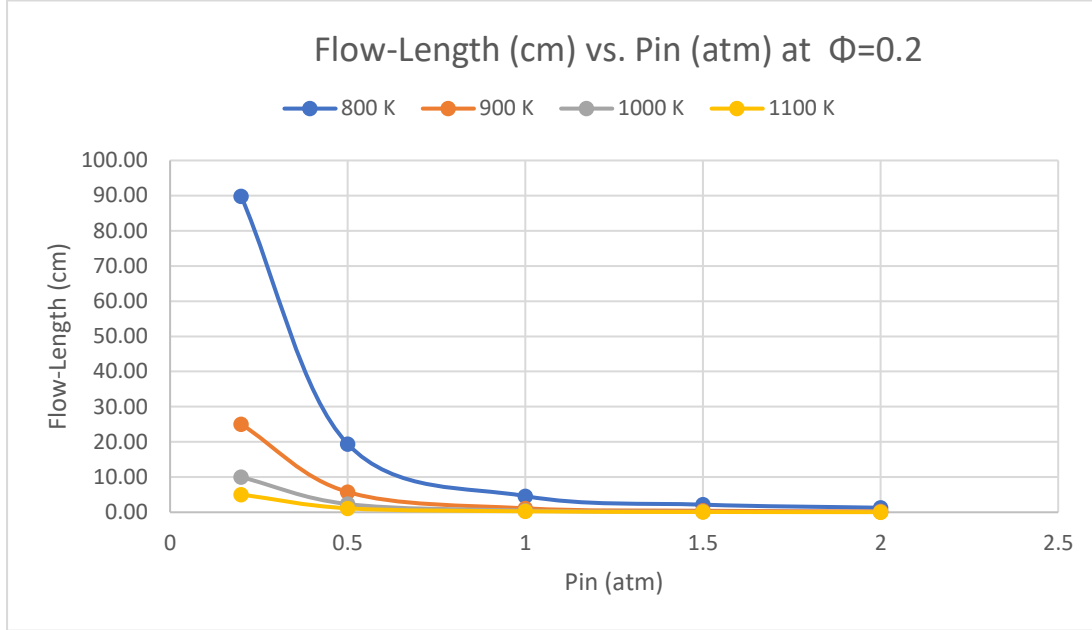


Figure 5 Flow-length vs. Pressure for $\phi = 0.2$

For $\phi = 0.5$

At $\phi = 0.5$	Temperature (T_{in}) (K)				
Pressure (P_{in}) (atm)	800 K	1000 K	1200 K	1500 K	
0.2	41.9	3.03	0.86	0.34	Flow- Length (cm)
0.5	9.75	0.63	0.18	0.05	
1	3.32	0.18	0.04	0.02	
2	1.07	0.05	0.01	0	

Table 3 Table of flow-length for $\phi=0.5$

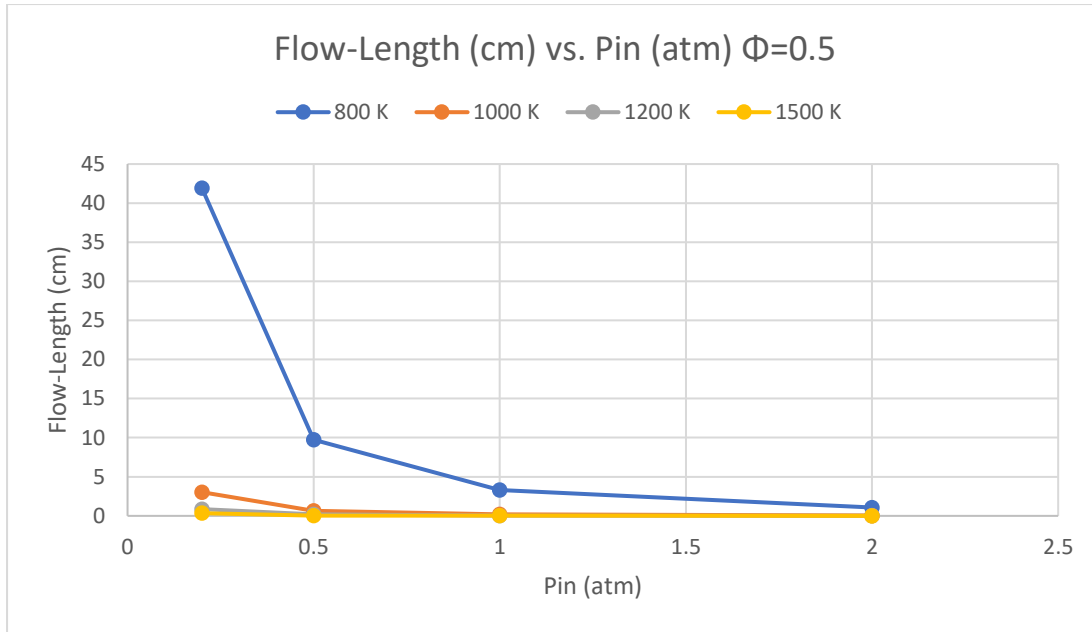


Figure 6 Flow-length vs. Pressure for $\phi=0.5$

For $\phi = 1$

At $\phi = 1$	Temperature (T_{in}) (K)				
Pressure (P_{in}) (atm)	800 K	1000 K	1200 K	1500 K	
0.2	38.16	9.05	3.17	1.04	Flow- Length (cm)
0.5	2.10	0.47	0.15	0.05	
1	0.36	0.08	0.02	0.01	
2	0.07	0.02	0.00	0.00	

Table 4 Table of flow-length for $\phi=1$

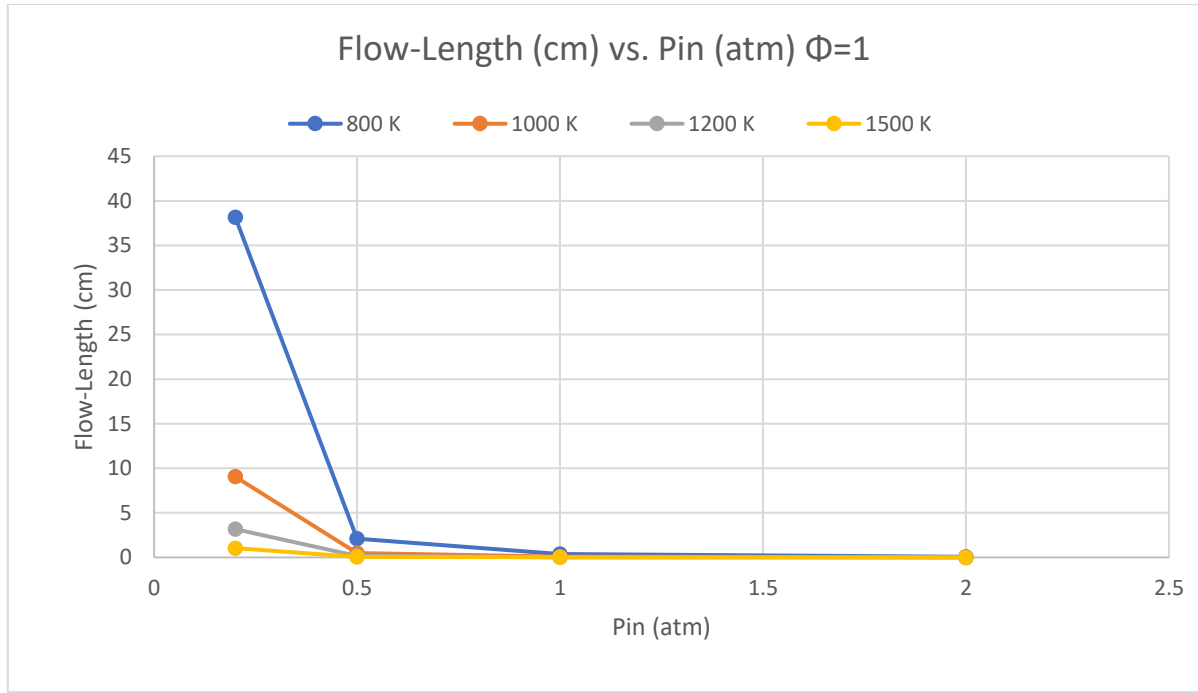


Figure 7 Flow-length vs. Pressure for $\phi=1$

The effect of ϕ , on the flow-length is tabulated below. Here ϕ was varied by keeping the P_{in} and T_{in} constant as 0.2 atm and 1000 K respectively.

For constant T_{in} and P_{in}

At $T_{in} = 1000$ K and $P_{in} = 0.2$ atm								
Flow-length (cm)	24.81	15.14	10.00	3.10	2.43	2.22	2.14	2.10
ϕ (ϕ)	0.1	0.15	0.2	0.5	0.75	1	1.25	1.5

Table 5 Variation of flow-length on ϕ , by keeping constant T_{in} and P_{in}

Discussion

From the graph above, we can observe that at a particular value of equivalence ratio, with increasing pressure and temperature, the flow-length required for 99 percent reaction decreases. Increasing pressure reduces the mean free path of molecules, which increase the probability of collisions of molecules with other molecules. Thus, increasing pressure increses the reaction rate, which leads to a lesser flow-length.

With an increase in temperature, the internal energy of the molecules increases. Thus, reducing the activation energy barrier, and resulting into a faster reaction. Thus, the reaction gets complete in lesser time, decreasing the residence time. So, the species spent a less time inside the reactor, hence the flow-length gets reduced. Moreover, with an increase in kinetic energy, the probability of collision increases, which also results into a faster reaction.

With an increase in equivalence ratio (ϕ), the flow length is found to be decreasing. Moreover, the rate of decrease of flow-length is found to be reducing significantly, as we increase ϕ beyond 0.75. With an increase in ϕ , the concentration of fuel increases, which would increase the rate of reaction. thus reducing the flow-length for 99% completion of reaction.

For practical application, a maximum possible values for T_{in} , P_{in} and ϕ should be selected to have a minimum possible flow-length. However, T_{in} and P_{in} are bound by material of the equipment. Also, by increasing ϕ , the amount of pollutants also increase. So, the equivalence ratio ϕ , should be selected as minimum as possible.

Conclusion

Increasing the inlet pressure and temperature or ϕ will reduce the flow length for 99 per cent complete combustion. While designing the plug-flow reactor, the materials of equipment should be chosen, such that they could operate at some maximum possible T_{in} and P_{in} . To meet the environment norms, the amount of pollutants like NO and CO should be controlled by keeping the equivalence ratio ϕ as minimum as possible.