CHE 321 321 Project

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1. Design Basis

Inlet Information:

- Inlet Information:
- Total Flowrate initial:

$$F_{To} = 172.8\frac{kmol}{h} * \frac{1000mol}{1kmol} * \frac{1h}{3600s} = 48\frac{mol}{S} \quad (1)$$

- Temperature:

$$400 + 273.15 = 673.15\ K \quad (2)$$

- Assumptions:

Assumptions:

1. Steady state

(1) **Catalytic Cracking Reactions for parraffins**

- Here are the given reactions and reaction rates:

$P8 + H2 \leftrightarrow P7 + P1$	$r_1 = k_1 (P_{p8})$
$P8 + H2 \leftrightarrow P6 + P2$	$r_2 = k_2 (P_{p8})$
$P8 + H2 \leftrightarrow P5 + P3$	$r_3 = k_3 (P_{p8})$
$P8 + H2 \leftrightarrow 2P4$	$r_4 = k_4 (P_{p8})$
$P7 + H2 \leftrightarrow P6 + P1$	$r_5 = k_5 (P_{p7} - P_{p6} P_{p1}/ K_5)$
$P7 + H2 \leftrightarrow P5 + P2$	$r_6 = k_6 (P_{p7} - P_{p5} P_{p2}/ K_6)$
$P7 + H2 \leftrightarrow P4 + P3$	$r_7 = k_7 (P_{p7} - P_{p4} P_{p3}/ K_7)$
$P6 + H2 \leftrightarrow P5 + P1$	$r_8 = k_8 (P_{p6} - P_{p5} P_{p1}/ K_8)$
$P6 + H2 \leftrightarrow P4 + P2$	$r_9 = k_9 (P_{p6} - P_{p4} P_{p2}/ K_9)$
$P6 + H2 \leftrightarrow 2P3$	$r_{10}=k_{10} (P_{P6} – P_{P3}^2 /K_{10})$
$P5 + H2 \leftrightarrow P4 + P1$	$r_{11}=k_{11} (P_{P5} – P_{P4} P_{P1}/K_{11})$
$P5 + H2 \leftrightarrow P3 + P2$	$r_{12}=k_{12} (P_{P5} – P_{P3} P_{P2}/K_{12})$
$P4 + H2 \leftrightarrow P3 + P1$	$r_{13}=k_{13} (P_{P4} – P_{P3} P_{P1}/K_{13})$
$P4 + H2 \leftrightarrow 2P2$	$r_{14}=k_{14} (P_{P4} – P_{P2}^2 /K_{14})$
$P3 + H2 \leftrightarrow P2 + P1$	$r_{15}=k_{15} (P_{P3} – P_{P2} P_{P1}/K_{15})$
$P3 \leftrightarrow N3 + H2$	$r_{21} = k_{21} (P_{p3})$
$P4 \leftrightarrow N4 + H2$	$r_{22} = k_{22} (P_{p4})$
$P5 \leftrightarrow N5 + H2$	$r_{23} = k_{23} (P_{p5})$
$P6 \leftrightarrow N6 + H2$	$r_{24} = k_{24} (P_{p6})$
$P7 \leftrightarrow N7 + H2$	$r_{25} = k_{25} (P_{p7})$
$P8 \leftrightarrow N8 + H2$	$r_{26} = k_{26} (P_{p8})$
$N6 \leftrightarrow A6 + 3H2$	$r_{31} = k_{31} \ (P_{N6}^{1.4})$
$N7 \leftrightarrow A7 + 3H2$	$r_{32} = k_{32} \ (P_{N7}^{1.4})$
$N8 \leftrightarrow A8 + 3H2$	$r_{33} = k_{33} \ (P_{N8}^{1.4})$

2. Procedure

- k_i values can be calculated using this equation:

$$k_i = A_i * \ e^{\frac{-E_i}{RT}} \tag{3}$$

- As the reactions are dependent on partial pressure, we can use this equation:

$$P_{pi} = \frac{F_{pi}}{F_{Tot}} * \ P_o \tag{4}$$

(1) **ODE for Mole Balances**

$$\frac{dF_{\text{P1}}}{dZ} = A_{\text{c}} * (r_1 + r_5 + r_8 + r_{11} + r_{13} + r_{15}) \tag{5}$$

$$\frac{dF_{\text{P2}}}{dZ} = A_{\text{c}} * (r_2 + r_6 + r_9 + r_{12} + 2 * r_{14} + r_{15}) \tag{6}$$

$$\frac{dF_{\text{P3}}}{dZ} = A_{\text{c}} * (r_3 + r_7 + 2 * r_{10} + r_{12} + 2 * r_{14} + r_{15}) \tag{7}$$

$$\frac{dF_{\text{P3}}}{dZ} = A_{\text{c}} * (r_3 + r_7 + 2 * r_{10} + r_{12} + r_{13} - r_{15} - r_{21}) \tag{8}$$

$$\frac{dF_{\text{P4}}}{dZ} = A_{\text{c}} * (2 * r_4 + r_7 + r_9 + r_{11} - r_{13} - r_{14} = r_{22}) \tag{9}$$

$$\frac{dF_{\text{P5}}}{dZ} = A_{\text{c}} * (r_3 + r_6 - r_8 - r_{11} - r_{12} - r_{23}) \tag{10}$$

$$\frac{dF_{\text{P6}}}{dZ} = A_{\text{c}} * (r_2 + r_5 - r_8 - r_9 - r_{10} - r_{24}) \tag{11}$$

$$\frac{dF_{\text{P7}}}{dZ} = A_{\text{c}} * (r_1 - r_5 - r_6 - r_7 - r_{25}) \tag{12}$$

$$\frac{dF_{\text{P8}}}{dZ} = A_{\text{c}} * (-r_1 - r_2 - r_3 - r_4 - r_{26}) \tag{13}$$

$$\frac{dF_{\text{N3}}}{dZ} = A_{\text{c}} * (r_{21}) \tag{14}$$

$$\frac{dF_{\text{N4}}}{dZ} = A_{\text{c}} * (r_{22}) \tag{15}$$

$$\frac{dF_{\text{N5}}}{dZ} = A_{\text{c}} * (r_{23}) \tag{16}$$

$$\frac{dF_{\text{N6}}}{dZ} = A_{\text{c}} * (r_{\text{24-31}}) \tag{17}$$

$$\frac{dF_{\text{N7}}}{dZ} = A_{\text{c}} * (r_{\text{25-32}}) \tag{18}$$

$$\frac{dF_{\text{N8}}}{dZ} = A_{\text{c}} * (r_{\text{26-32}}) \tag{19}$$

$$\frac{dF_{\text{A6}}}{dZ} = A_{\text{c}} * (r_{31}) \tag{20}$$

$$\frac{dF_{\text{A7}}}{dZ} = A_{\text{c}} * (r_{32}) \tag{21}$$

$$\frac{dF_{\text{A8}}}{dZ} = A_{\text{c}} * (r_{33}) \tag{22}$$

$$\frac{dF_{\text{H2}}}{dZ} = A_{\text{c}} * (-r_1 - r_2 - r_3 - r_4 - r_5 - r_6 - r_7 - r_8 - r_9 - r_{10} - r_{11} \\ -r_{12} - r_{13} - r_{14} - r_{15} + r_{21} + r_{22} + r_{23} + r_{24} + r_{25} + r_{31} + r_{32} + r_{33}) \tag{23}$$

(2 **ODE for Pressure Drop**

- To setup the ODE for pressure, I used 5-24 (Ergun Equation):

$$\frac{dP}{dZ} = \beta \frac{P}{p} \frac{T}{T} \frac{F_{\text{total}}}{F_{\text{T}}} \tag{24}$$

- Next, to calculate β using 5-25:

$$\beta = \frac{G(1-\psi)}{\rho_0 g_{\text{c}} D_{\text{p}} \psi^3} (\frac{150(1-\psi}{D_{\text{p}}} + 1.75G) \tag{25}$$

- Where G is the $\frac{\text{mass flow rate}}{\text{cross-sectional area}} \implies$

$$G = \frac{48 \text{ mol}}{1 \text{ s}} (\frac{0.02897 \text{ kg}}{1 \text{ mol}})(\frac{1}{0.0016619\text{m2}} = 836.7 \frac{\text{kg}}{\text{s*m2}} \tag{26}$$

- Area (A_c) was calculated using the $A_c = \pi\ r^2$ and using the radius found from the tube diameter and wall thickness

$$r = (.05m - (2 * .002)\, m)\,/2 = 0.023m \tag{27}$$

$$A_c = \pi * (.023)^2 = 0.0016619\ m^2 \tag{28}$$

- As we know the void fraction and D_ρ ($\psi = 0.45$ and $D_\rho = 0.002$), we can then find the ρ_0 and μ at the our inlet temperature at 673.15K

$$\rho_0 = .5252 \frac{kg}{m^3} \qquad \mu = 3.25 * 10^{-25} \frac{kg}{s * m} \tag{29}$$

- Finally, we can calculate $\beta = 69540$

(3) **ODE for Temperature**

- First, we need to calculate the Cpi values using the Shomate equation:

$$C_{Pi} = A + BT + CT^2 + DT^3 \tag{30}$$

- We will use the values of A,B,C,D to solve for the temperature using 11-1.3

$$\frac{dT}{dZ} = \frac{-U_a\,(T - T_a) + \Sigma\,(-r_i) * \Delta H_{ri}}{\Sigma F_i C_{pi}} * A_c \tag{31}$$

- In this case, (i) goes from P1-P8, N3-N8, A6-A8
- Also, in the co-current exchange system, I used 11-1:

$$\frac{dT_a}{dZ} = \left[\frac{Ua\,(T - T_a)}{m_{oil}\ * C_{Poil}}\right] * A_c \tag{32}$$

$$m_{oil}\ = 19.443 \frac{kg}{s} \tag{33}$$

(4) **MATLAB Variables**

$$X\,(1) = F_{P1} \tag{34}$$

$$X\,(1) = F_{P2} \tag{35}$$

$$X\,(3) = F_{P3} \tag{36}$$

$$X\,(4) = F_{P4} \tag{37}$$

$$X\,(5) = F_{P5} \tag{38}$$

$$X\,(6) = F_{P6} \tag{39}$$

$$X\,(7) = F_{P7} \tag{40}$$

$$X\,(8) = F_{P8} \tag{41}$$

$$X\,(9) = F_{N3} \tag{42}$$

$$X\,(10) = F_{N4} \tag{43}$$

$$X\,(11) = F_{N5} \tag{44}$$

$$X\,(12) = F_{N6} \tag{45}$$

$$X\,(13) = F_{N7} \tag{46}$$

$$X\,(14) = F_{N8} \tag{47}$$

$$X\,(15) = F_{A6} \tag{48}$$

$$X\,(16) = F_{A7} \tag{49}$$

$$X\,(17) = F_{A8} \tag{50}$$

$$X\,(18) = F_{H2} \tag{51}$$

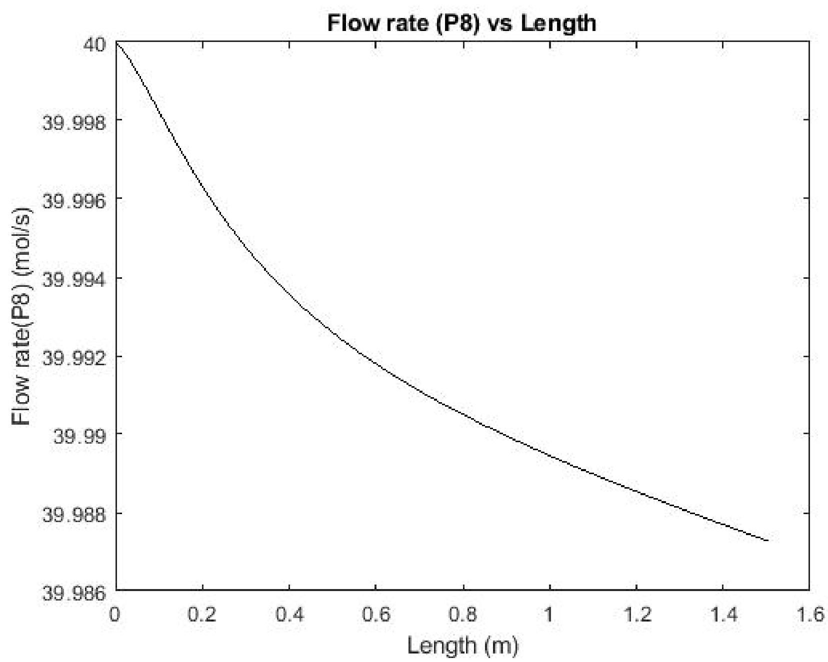
$$X\,(19) = T_{Gas/Feed} \tag{52}$$

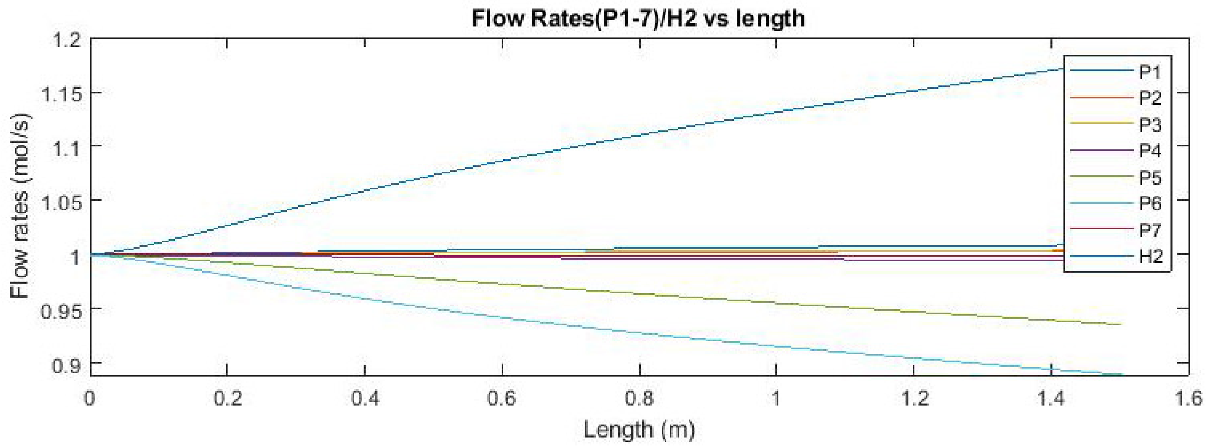
$$X\,(20) = T_{Oil} \tag{53}$$

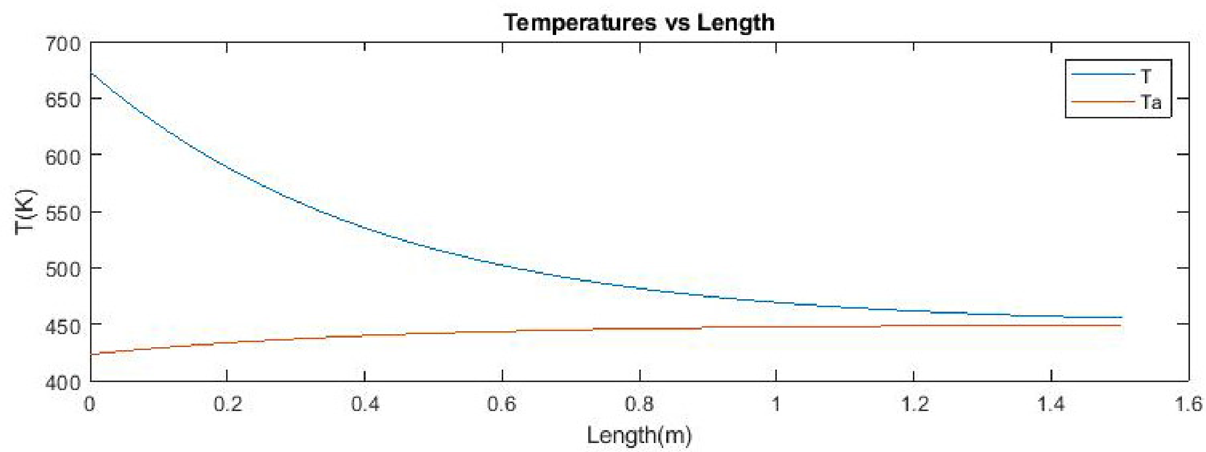
$$X\,(21) = Pressure \tag{54}$$

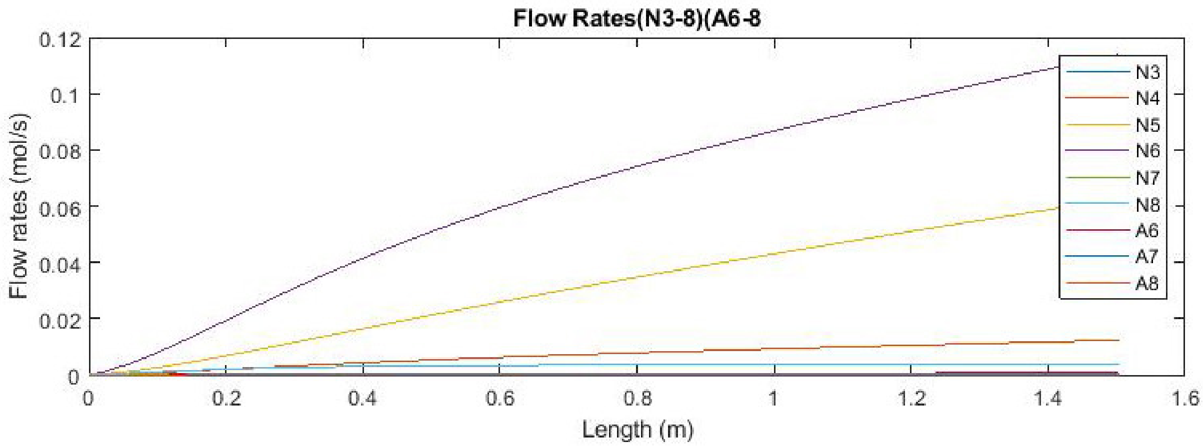
3. Results

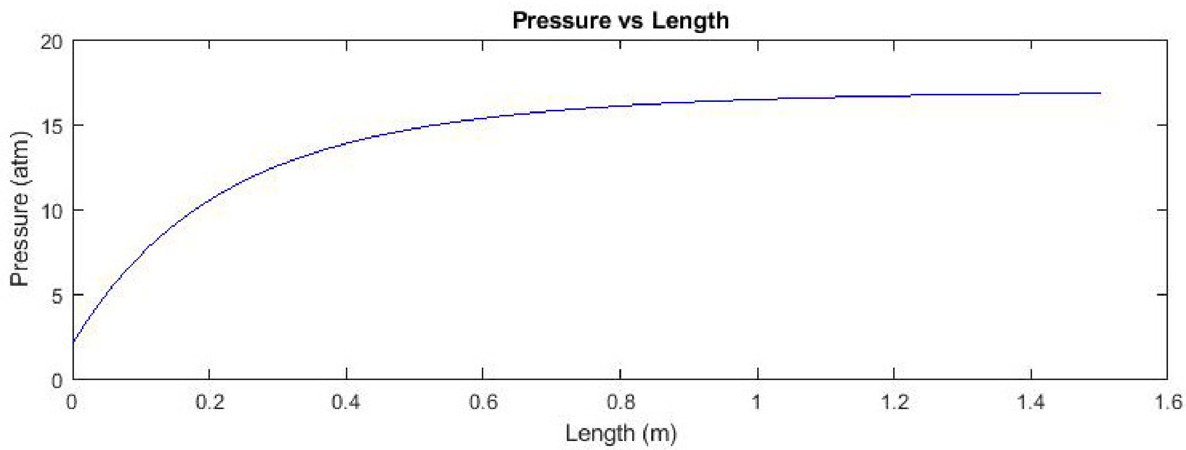
(1) **Graphs**




Flow Rates(P1-7)/H2 vs length
Flow rates (mol/s)
Length (m)
P1
P2
P3
P4
P5
P6
P7
H2
1.2
1.15
1.1
1.05
1
0.95
0.9
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6


Temperatures vs Length
T(K)
Length(m)
T
Ta
700
650
600
550
500
450
400
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6





(2) **Calculations**

$$x = \frac{F_{P8o} - F_{P8}}{F_{P8o}} = \frac{40\frac{mol}{s} - 39.9872\frac{mol}{s}}{40\frac{mol}{s}} = 0.00032 \text{ (Conversion Rate \%)} \quad (55)$$

(3) **Counter-current Heat Exchanger**

For the analysis of part 1 with counter-current heat exchanger:

1. Run a trial/error analysis of the script in order to find the temperature of the exiting coolant.
2. With our initial guess of the temperature initially, we can solve $\frac{dT}{dZ}$

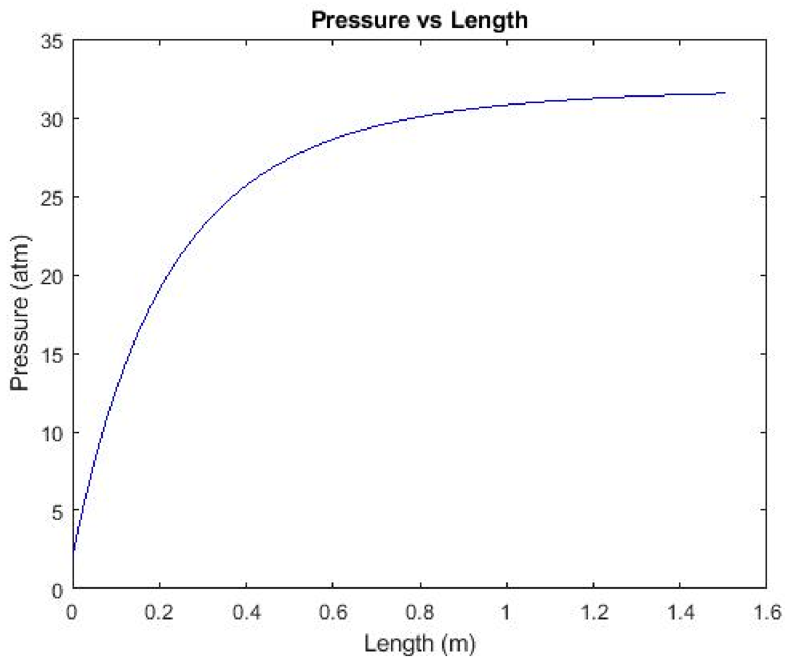
$$\frac{dT_a}{dZ} = \left(\frac{Ua\,(T_a - T)}{m_c * C_{Pc}}\right) * A_c \quad (56)$$

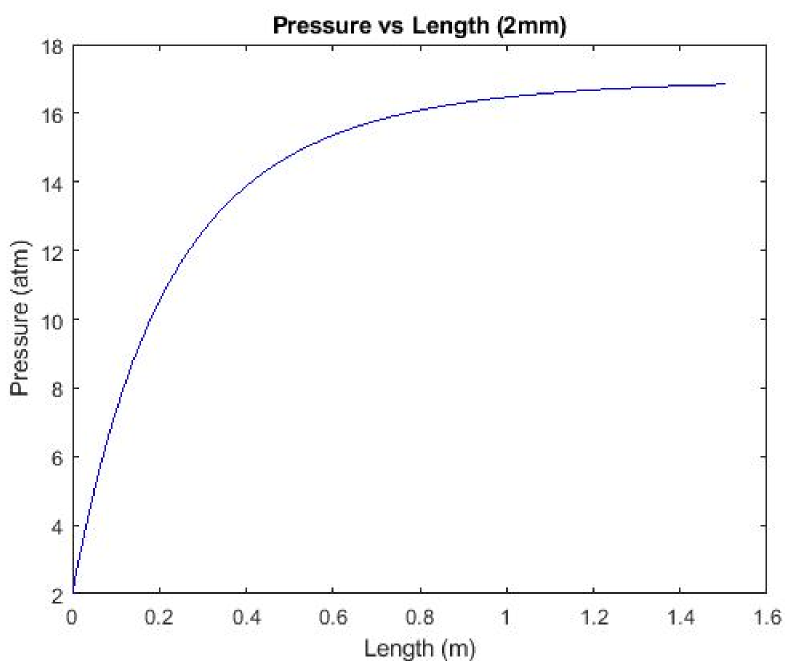
3. The temperature was $\approx$ 452K

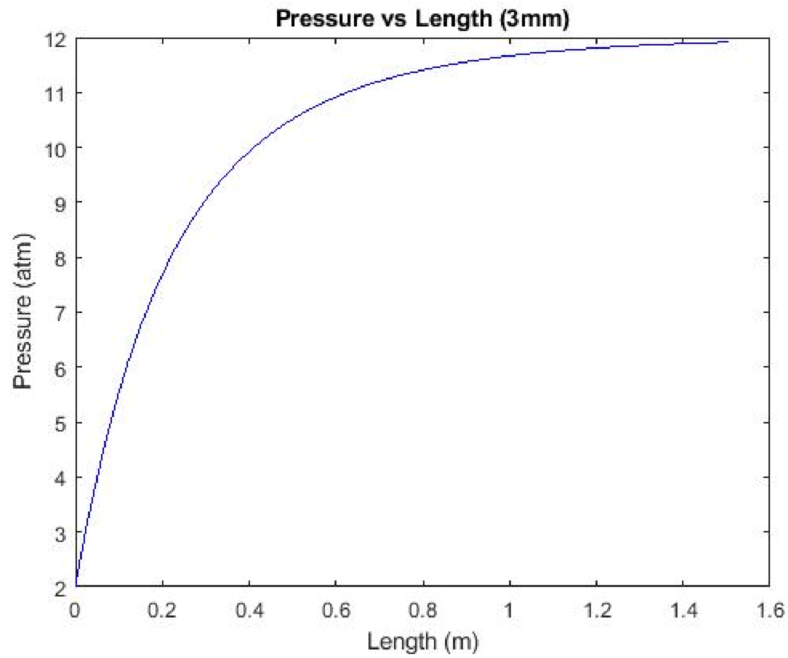
(4) **Different Particle Sizes (1-4 mm)**

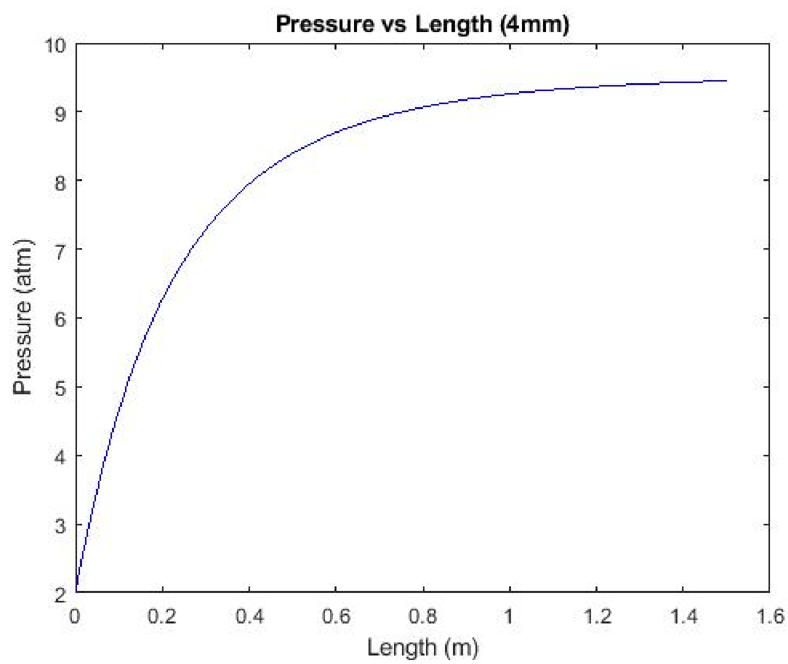
1. 1mm: $\beta = 139214$
2. 2mm: $\beta = 69544$

3. 3mm: $\beta = 46348.47$
4. 4mm: $\beta = 34766$



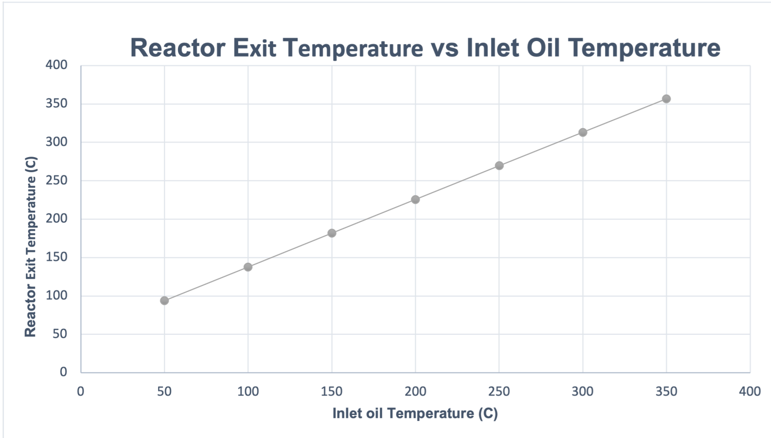


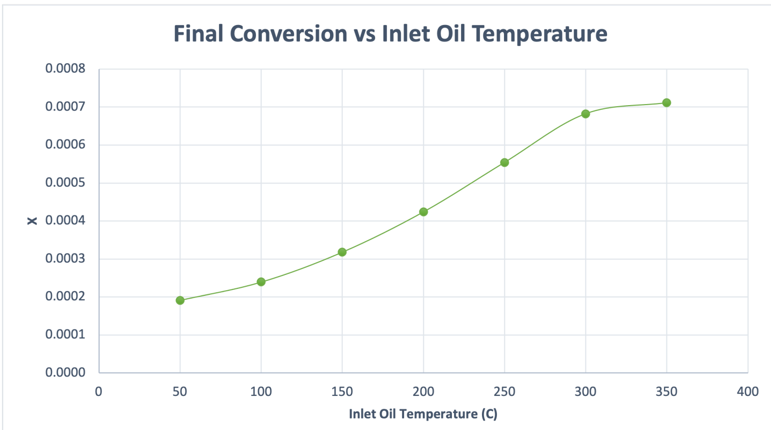




(5) **Inlet Oil Temperature**

Inlet oil temperature (50, 100, 150, 200, 250, 300 and 350C) as a function of the reactor exit temperature and final conversion (for 2 mm particle size).





4. Conclusion/Recommendations

(1) Design Change

We will reduce the temperature of the reactor and hence the conversion by using a coolant with a low temperature, in order to maximize conversion. We can do this by setting the inlet temperature of the oil from between 300 and 350 degrees.

(2) Concerns

1. Explosions from chemical reactions due to overpressure or due to release of energy (for example from H2)
2. Being exposed to high temperatures and stress from the reactor
3. If this reactor was being built, making sure of human-error when building it
4. Thermal runaway, which can lead to reactions being screwed up due to high temperature