DSN ENGINEERING: CONCEPTUAL REACTOR DESIGN FOR A NEW ACYRLIC ACID PLANT

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DSN ENGINEERING

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Abbreviations

AA	Acrylic Acid
CAPEX	Capital Expenditure
FBR	Fluidised Bed Reactor
LFL	Lower Flammability Limit
LMTD	Log Mean Temperature Difference
moc	Minimum Oxygen Concentration
OPEX	Operating Expenditure
PBR	Packed Bed Reactor
PFD	Process Flow Diagram
UFL	Upper Flammability Limit

Nomenclature

A_{ht}	Area of Heat Transfer	m^2
C_p	Heat Capacity	J / (mol • K)
D	Diameter Of Reactor	m
D_s	Shell Diameter	m
E_i	Activation Energy of Reaction i	kJ / kmol
F_i	Flowrate of component i	Kmol / hr
ΔH_{RX}	Enthalpy Change of Reaction	kJ / mol
$k_{0,I}$	Pre-exponential constant for reaction i	Kmol / m^3
L	Height of Reactor	m
Mr_{avg}	Average Molecular Mass of mixture	Kg / kmol
N_t	Total Number of Tubes	n/a
p_{oxygen}	Partial Pressure of Oxygen	kPa
$p_{polypropene}$	Partial Pressure of Propylene	kPa
p_{Total}	Total Pressure in Reactor	kPa
Q	Energy Released from Reaction	kJ / hr
R	Ideal Gas Constant (8.314)	kJ / (kmol • K)
T_{FBR}	Temperature of FBR	K
T_{PBR}	Temperature of PBR	K
$T_{Cool, in}$	Inlet Temperature of cooling fluid	K
$T_{Cool, Out}$	Outlet Temperature of cooling fluid	K
U	Overall Heat Transfer Coefficient	kJ / (hr • m^2 • K)
u_s	Superficial Gas Velocity	m / s
V	Reaction Volume	m^3
$X_{Propylene}$	Conversion Of Propylene	n/a
Y_{AA}	Yield of Acrylic Acid	n/a
ρ_{gas}	Density of Gas Mixture	Kg / m^3

Abstract

DSN has developed a new catalyst that allows the production of acrylic acid (AA) directly from propylene. The aim of this paper is to look for a replacement reactor; choosing between a fluidised bed reactor (FBR) or a packed bed reactor (PBR).

All the calculations and the graphs in this paper were made using MATLAB. A system of ordinary differential equations, produced from the mole and energy balances, were solved simultaneously.

After determining the specifications of both reactors, it was concluded that the PBR was the more appropriate choice of reactor. Firstly, its diameter and height were smaller than the FBR, and thus more in-line with the dimensions of previous reactors used by DSN. Smaller reactors would not only save space, but also make it much easier to retrofit the design into existing DSN facilities. Furthermore, the PBR surpassed the production quota with 45,300 tonnes per year of acrylic acid. This was significantly higher the production rate of the FBR (41,500 tonnes per year). As well as this, The PBR had a significantly higher yield of AA at 88.5%, compared to 80.0% yield of AA for the FBR. The two reactors showed similar conversion rates of propylene, of around 89%. The mass flowrates into each reactor were similar, with the PBR requiring slightly more nitrogen (1500 kmolh^{-1}, compared to 1340 kmolh^{-1} for FBR). The only major disadvantage of using the PBR was that it used significantly more cooling tubes to achieve the necessary heat transfer area. However, considering all the other benefits of the PBR, it is still the most appropriate reactor for DSN to use in any future plants.

Design Brief and Aims

Currently, DSN manufactures its Acrylic Acid (AA) through a two-step process, in which propylene is oxidised to acrolein (step 1) and then oxidised to AA (step 2). However, a new catalyst has been developed, enabling the manufacture of AA directly from propylene.

There are two key advantages of using the new catalyst. Firstly, only one reactor is required, as the new catalyst allows for a one-step process. DSN hopes that this will reduce equipment and operating costs. Secondly, the new method eliminates acrolein, which is a necessary intermediate product in the two-step process. Acrolein is a dangerous substance for many reasons. Breathing acrolein can cause build-up of fluid in the lungs, coughing and shortness of breath. Exposure irritates the skin, damages the eyes and, in high concentrations, can cause death. Beyond medical issues, it is also flammable and reactive, making it an explosion hazard (New Jersey Department of Health and Senior Services, 2005). For these reasons, DSN believes that the new process will almost certainly improve process safety. For the new process, three reactions take place simultaneously over the 3 reactions in Table 1. The mixture exiting the reactor is then separated. For the new process, three reactions take place simultaneously over the catalyst presented in Table 1. The mixture exiting the reactor is then separated.

Table 1 – Showing the reactions taking place in the new process. These are the only reactions taking place across the new catalyst.

	Molecular Formula	Written Formula
1	$C_3H_6 + 1.5\ O_2 \rightarrow C_3H_4O_2 + H_2O$	Propylene + Oxygen $\rightarrow$ AA + Water
2	$C_3H_6 + 2.5\ O_2 \rightarrow C_2H_4O_2 + CO_2 + H_2O$	Propylene + Oxygen $\rightarrow$ Acetic Acid + Water + Carbon Dioxide
3	$C_3H_6 + 4.5\ O_2 \rightarrow 3\ CO_2 + 3\ H_2O$	Propylene + Oxygen $\rightarrow$ Carbon Dioxide + Water

The aim of this paper is to assess the conceptual design for a reactor using this new, single-step method. Each year, the plant is expected to operate 8000 hours and produce 40,000 tons of AA. The overall conversion of propylene must be at least 85%, and the overall yield of AA must be at least 80%. Typically, DSN uses a fluidised bed reactor (FBR) for this process, however the use of a packed bed reactor (PBR) will be considered also. The ideal specifications will be calculated for both reactor types, and the advantages and disadvantages of each will be discussed. Furthermore, as DSN already operates multiple AA plants using the two-step process, the viability of retrofitting existing plants will also be explored.

Design Methods, Results and Calculations

To determine the dimensions of both the fluidised bed reactor and the packed bed reactor, a system of ordinary differential equations as well as many other calculations needed to be solved. MATLAB was the primary tool used to make these calculations. The graphs and results were optimised using an iterative trial-and-error method. For example, initial conditions were changed within each reactor, and then other variables were subsequently changed to ensure the dimensions and specifications of the reactor agree with the given constraints.

The three reactions listed in Table 1 are assumed to be irreversible, and the only reactions taking place during the process. Other components moving through the reactors include nitrogen, which is assumed to be completely inert. Other than nitrogen and the components included in the three reactions, there is nothing else passing through the catalyst side of each reactor.

When designing the reactors, a mole balance is setup into differential equations, where it is then analysed for the changes in the different flowrates of each component. The Fluidised Bed Reactor operates under isothermal conditions; therefore, no energy balance equation is needed for this reactor. The PBR, on the other hand requires an energy balance (see Equation 10).

From Mole Balance:
$$F(V) - F(V + \Delta V) + r_j \Delta V = 0 \qquad \text{Eq.1}$$

Rearranging Equation 1 :
$$\frac{dF}{dV} = r_j \qquad \text{Eq.2}$$

Equation 3 is valid within a temperature range of 250°C and 350°C and pressure range of 2 bara and 5 bara:

$$-r_i = k_{0,i} \times e^{\left(\frac{-E_i}{RT}\right)} \times p_{propylene} \times p_{oxygen} \qquad \text{Eq.3}$$

The values for the activation energy and pre-exponential factor can be found in Table 6 in the Appendix. Equations 20 to 22 in the Appendix show the full expressions for the above equation.

Once the balance equations are derived, the equations for each of the components can be determined. The following mole balances are valid for both the FBR and PBR:

Propylene:
$$\left(\frac{dF}{dV}\right) = r_1 + r_2 + r_3 \qquad \text{Eq.4}$$

Oxygen:
$$\left(\frac{dF}{dV}\right) = \left(\frac{3}{2}r_1\right) + \left(\frac{5}{2}r_2\right) + \left(\frac{9}{2}r_3\right) \qquad \text{Eq.5}$$

Acrylic Acid:
$$\left(\frac{dF}{dV}\right) = -r_1 \qquad \text{Eq.6}$$

Acetic Acid:
$$\left(\frac{dF}{dV}\right) = -r_2 \qquad \text{Eq.7}$$

Carbon Dioxide:
$$\left(\frac{dF}{dV}\right) = -r_2 - (3r_3) \qquad \text{Eq.8}$$

$$\left(\frac{dF}{dV}\right) = -r_1 - r_2 - (3r_3)$$

Eq.9

Equations 4 – 9 can be solved using the 'ode45' function in MATLAB, the results were as expected, with the flowrates changing with respect to reaction volume under isothermal conditions. The results can be seen in Figure 1 and Figure 2 below, which are the graphs for the FBR and PBR, respectively.
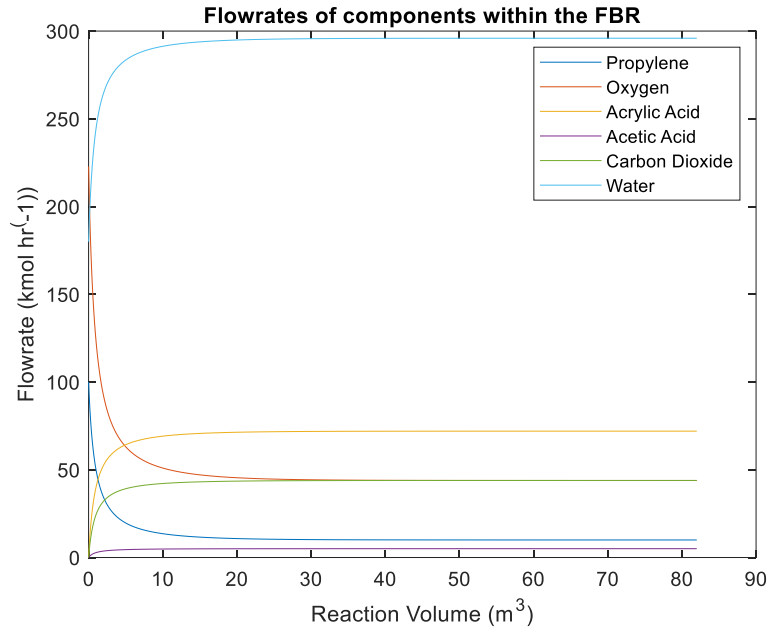

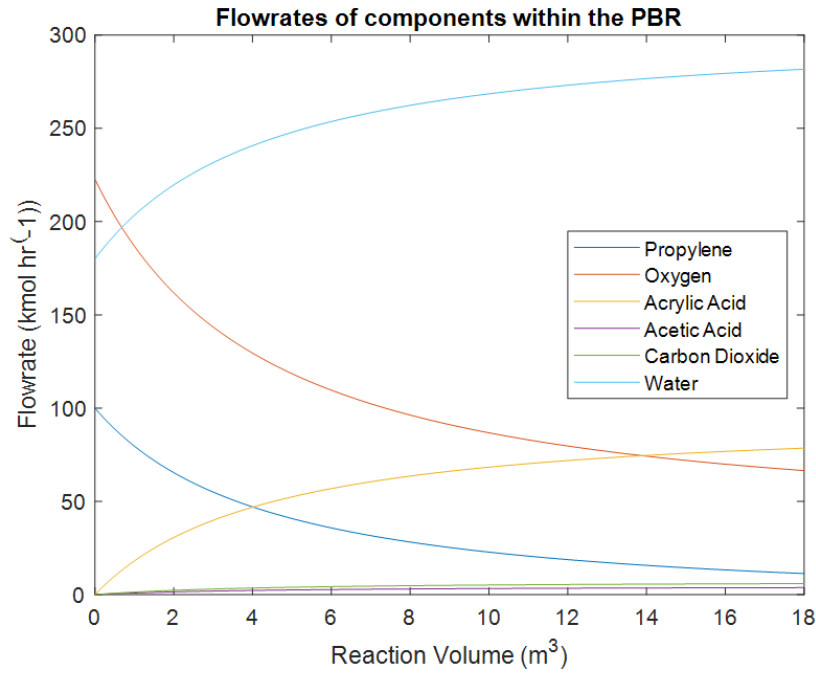*Figure 1: Change in Flowrates of the various components across the FBR*

Figure 2: Change in Flowrates of the various components across the PBR

For the PBR only, an energy balance equation is required:

$$\frac{dT}{dV} = \frac{\sum_{i=1}^{q} r_{ij}\,\Delta H_{rxij} - UA_{ht}(T - T_{PBR})}{\sum_{j=1}^{m} F_j\, C_{P_j}}$$

Eq.10

As the PBR is non-isothermal, the temperature change was graphed to ensure that the temperature difference between the reaction and the cooling fluid did not exceed 100K, the temperature is plotted via MATLAB, using the 'ode45' function to solve Equation 10. The results are shown in Figure 3:
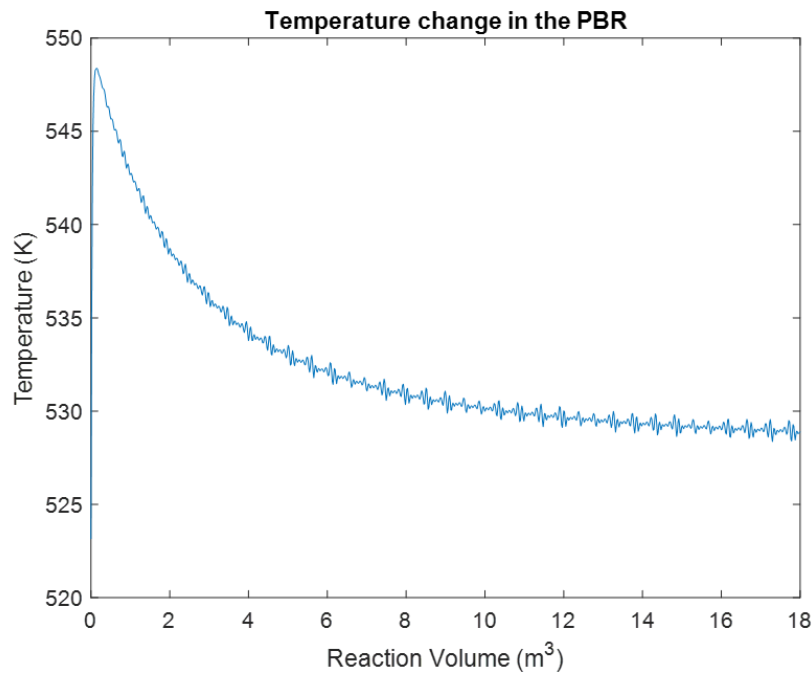

Figure 3: Temperature change in the tubes, within the PBR

Keeping the temperature within the 100K range was achieved by finding the optimum flowrate for the inert Nitrogen gas.

The temperature fluctuates within 100K of the value of T_{PBR}. Because the PBR is non-isothermal, there will be a heat loss to the surroundings, which is expressed by $UA_{ht}(T - T_{PBR})$ within Equation 10. The temperature difference was plotted, and it was observed that the graph's peaks and troughs were within the appropriate range, as can be observed in Figure 3.

The final flowrate values, which can be observed in Figure 1 and 2, were used to calculate the AA production per year which, assuming the reactors are run continuously for 8000 hours, meet the requirements. The results are presented in Table 2. Once the values for the flowrates are determined, the conversion of propylene and yield of AA can be calculated using Equations 11 and 12 respectively:

$$X_{\mathrm{Pr\,opylene}} = \frac{F_{0,\mathrm{Pr\,opylene}} - F_{\mathrm{Pr\,opylene}}}{F_{0,\mathrm{Pr\,opylene}}}$$

Eq.11

$$Y_{AA} = \frac{F_{Acrylic\ Acid}}{F_{0,\mathrm{Pr\,opylene}} - F_{\mathrm{Pr\,opylene}}}$$

Eq.12

Table 2 – Yearly production, propylene conversion and yield of AA for both reactors.

	Min. Requirement	FBR	PBR
AA Production (t/year)	40,000	41,500	45,300
Overall Conversion of Propylene (%)	85	90.0	88.7
Overall Yield of Acrylic Acid (%)	80	80.0	88.5

In order to determine the reactor dimensions, the heat transfer area must be determined. Equation 13 shows how to calculate the Log Mean Temperature Difference, assuming the system can be modelled as a counter-current heat exchange system.

$$LMTD = \frac{(T_{h,in} - T_{c,out}) - (T_{h,out} - T_{c,in})}{\ln\left(\frac{T_{h,in} - T_{c,out}}{T_{h,out} - T_{c,in}}\right)}$$

Eq.13

Using the LMTD and assuming the reactors are cylindrical, Equation 14 can be used to calculate the area of heat transfer (A_{ht}) required:

$$A_{ht} = \frac{Q}{(U \times LMTD)}$$

Eq.14

The area of heat transfer for both reactors can be found in the specification sheet (Table 3). The cooling for both reactors is modelled after a shell and tube counter-current heat exchanger. For the FBR, the cooling fluid travels through the tube side and the reactants and catalyst mixture will flow on the shell side, and vice versa for the PBR. Once the area of heat transfer is calculated, and a height of reactor is selected, the number of cooling tubes can be determined from equation 15:

$$N_t = \frac{A_{ht}}{l_{cool} \times \pi \times d_i}$$

Eq.15

For the FBR, It is assumed that the outer wall of the cooling tubes is the same temperature as the cooling fluid within the tubes. For the PBR, it is assumed that the inner walls of the tubes are the same temperature as the bulk cooling fluid. From the number of cooling tubes, the shell diameter can be calculated according to Equation 16.

$$D_s = 2\sqrt{\frac{N_t}{\pi} \times PR \times d_o} + 2d_o$$

Eq.16

The shell diameter for both reactors can be found in the specification sheet. For the FBR, a diameter to length ratio of 1:1.5 to 1:3 is required. This conceptual design narrowly fits into that constraint with a diameter to length ratio of 1:1.70. For the PBR, the calculated diameter to length ratio was 1:1.79, also within the given constraints; between 1:1.5 and 1:4.

Values for superficial gas velocity can be found in the specification sheet, these values were obtained from the molar flowrate via Equation 17:

$$\therefore u = \frac{\dot{V}}{A_{C.S,}} = \dot{n}\left(\frac{RT}{PA_{C.S.}}\right)$$

Eq.17

To ensure the safe operation of the reactors, the lower flammability limit of our component mixture had to be calculated via Equation 18, which then needs to be compared to Equation 19. The LFL_{mix} value must be lower than our moc. This ensures the mixture is not flammable, thus ensuring the process is safe.

$$\frac{1}{LFL_{mix}} = \sum_{i=1}^{n} \frac{y_i}{LFL_i} \qquad Eq.18$$

$$moc = LFL_{mix} \frac{moles\ of\ oxygen\ for\ complete\ combustion}{moles\ for\ fuel} \qquad Eq.19$$

Table 3: Specification Sheet

			Fluidised bed reactor	**Packed bed reactor**
	Type of Reactor			
Equipment dimensions				
	Height of reaction zone	m	7	6
	Shell diameter	m	4.133	3.327
	Heat exchange area	m^2	1368	3554
Tube side	Substance	-	Molten Salt	Catalyst and Reactants
	Number of tubes	-	1862	9429
	Type of pitch	-	Square	Square
	Tube diameter	m	0.0334	0.02
	Pitch ratio	-	2.5	1.5
	Superficial velocity (if applicable)	m/s	N/A	4.010
Shell side	Substance	-	Catalyst and Reactants	Molten Salt
	Superficial velocity (if applicable)	m/s	1.038	N/A
Operating conditions				
	Operating pressure	bara	2	2
	Inlet temperature, shell side	°C	302	243
	Outlet temperature, shell side	°C	302	243
	Inlet temperature, tube side	°C	200	255
	Outlet temperature, tube side	°C	250	255.73

Stream Table and Simplified Process Flow Diagram for FBR

Figure 4 – A simplified diagram depicting the FBR. Streams 6 and 7 are not listed in the stream table (Table 3). They represent the inlet and outlet cooling fluid.

Table 4 – Mass and Molar flowrates of components at different parts of the FBR.

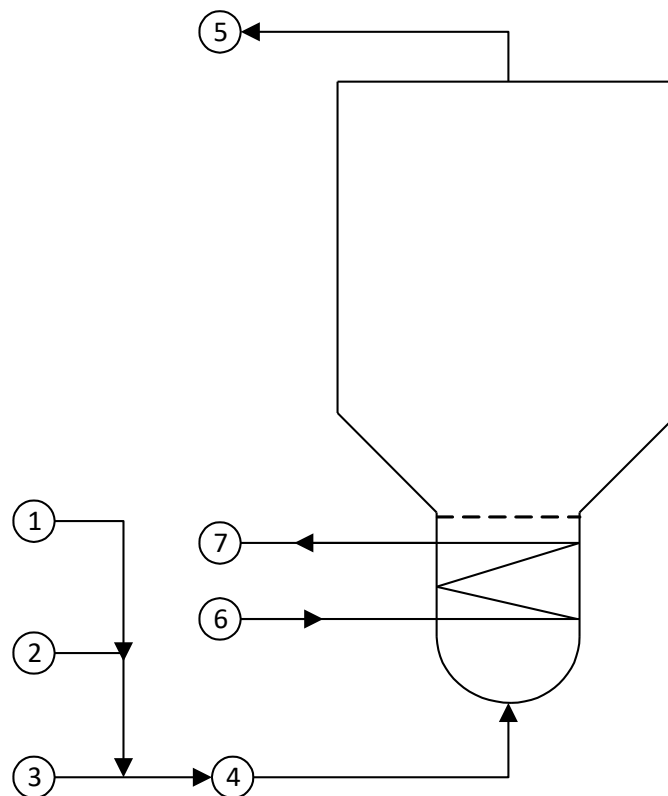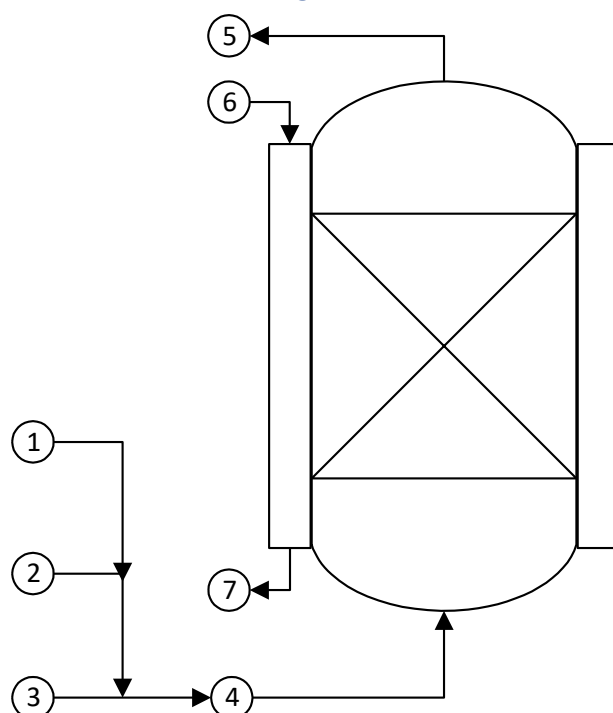| Stream Number	1 Air Inlet	2 Steam Inlet	3 Propylene	4 Reactor Inlet	5 Reactor Outlet
Mass Flow (kg / hr)	44600	3240	4200	52040	52040
Mole Flow (kmol / hr)	1561	180	100	1841	1809
Component Molar Flow Rate (kmol / hr)					
Propylene	0	0	100.00	100.00	10.00
Oxygen	222.80	0	0	222.80	43.89
Nitrogen	1338.15	0	0	1338.15	1338.15
Carbon Dioxide	0	0	0	0	43.91
Water	0	180.00	0	180.00	296.00
AA	0	0	0	0	72.01
Acetic Acid	0	0	0	0	5.03

Figure 5 – A simplified diagram depicting the PBR. Streams 6 and 7 are not listed in the stream table (Table 3). They represent the inlet and outlet cooling fluid respectively.

Table 5 – Mass and Molar flowrates of components at different parts of the PBR.

Stream Number	1	2	3	4	5
	Air Inlet	Steam Inlet	Propylene	Reactor Inlet	Reactor Outlet
Temperature (K)	523.15	523.15	523.15	523.15	528.88
Mass Flow (kg / hr)	49129.6	3240	4208	56577.6	56577.6
Mole Flow (kmol / hr)	1722.8	180	100	2002.8	1947.604
Component Molar Flow Rate (kmol / hr)					
Propylene	0	0	100	100	11.276
Oxygen	222.8	0	0	222.8	66.491
Nitrogen	1500	0	0	1500	1500
Carbon Dioxide	0	0	0	0	5.886
Water	0	180	0	180	281.727
AA	0	0	0	0	78.505
Acetic Acid	0	0	0	0	3.719

Discussion

One key advantage of using the new process is that, because it only has one step, only one reactor is required, unlike the former process which requires at least two reactors. Therefore, for the new process, placing multiple reactors in series or in parallel will not be considered.

As seen from Figure 1, the FBR requires a very small volume before is the reaction is essentially complete. For example, at around 30m^3 through the reactor, the flowrate of all components has

become constant, as indicated by the linear shape. However, the reaction volume must be made much larger, as it needs to match the reaction volume derived from equation 16. Making these values match was done through trial-and-error iteration. Figure 2 shows that, within the PBR, the reactions are not complete by the final reaction volume, as no lines on the graph are linear at any point. Despite this, it was not necessary to increase the reaction volume, as by this point, it had already achieved all requirements. Given that the FBR requires a much greater reaction volume ($82m^3$ compared to $18m^3$) and has a much greater pitch ratio (2.5 compared to 1.5), one obvious advantage that the PBR has is reactor dimensions. The FBR shell diameter (4.13m) is slightly larger than previous FBRs built by DSN (less than 4m). The FBR height is also at the maximum permissible value of 7m, whereas the PBR is slightly shorter at 6m. Altogether the PBR has a much smaller area footprint, and thus a smaller CAPEX. The FBRs large size may also be troublesome if DSN wishes to retrofit existing plants.

One advantage that the FBR was thought to have over the PBR was that extra nitrogen was not required. However, this was not the case, as the FBR required extra nitrogen in order to achieve an appropriate superficial gas velocity. When air at standard composition was pumped through the reactor, superficial velocity was below the minimum fluidisation velocity (1 ms^{-1}). An extra 500 kmolh^{-1} of nitrogen had to be added to the air inlet stream, which raised the superficial gas velocity to 1.04 ms^{-1}. The nitrogen flowrate was chosen as the appropriate variable to change, as nitrogen is inert, and would have a very small effect on the reactions. Despite the need for extra nitrogen to be added to the FBR air inlet stream, the total extra nitrogen needed is less than what is required for the PBR. The FBR requires an extra 500 kmolh^{-1} to be added to the air inlet stream, whereas the PBR requires 660 kmolh^{-1} to the air inlet stream. Therefore, the FBR still has a slight advantage in this regard, as the OPEX would not be as high.

An issue specific to the FBR is that a sudden loss of pressure would lead to a reduction in surface area of the bed. The superficial gas velocity within the FBR (1.04 ms^{-1}) is only narrowly above the minimum fluidization velocity (1 ms^{-1}), and therefore the risk of the FBR loosing fluidization is very high. Firstly, this is an inconvenience, as restarting the reactor would be difficult. Secondly, as the reaction is highly exothermic, a sudden restriction in heat transfer would lead to the temperature rapidly increasing. This could lead to a more serious problem: a runaway reaction (Trambouze & Euzen, 2004) or the catalyst coking-up. Therefore, a back-up source of gas may be necessary to ensure such a problem does not arise, adding to the CAPEX and OPEX of using the FBR.

Another key disadvantage of an FBR is high particle entrapment. It is likely that some solid catalyst particles will be entrapped within the fluid and be transported out of the reactor and further downstream. Therefore, use of an FBR will require additional separation equipment to remove any catalyst particles. This increases both the CAPEX and OPEX of using an FBR. The constant motion of the solid particles in an FBR also leads to a tremendous amount of erosion of internal components, such as the cooling tubes, which then need to be replaced. This drastically increases the maintenance cost and reduces available operating time (Trambouze & Euzen, 2004). Despite the PBR requiring far more cooling tubes than the FBR, a PBR would probably still have lower CAPEX, OPEX and maintenance costs.

The primary purpose of this activity was to improve plant safety through eliminating an intermediate step that produced acrolein. Although this process has successfully done this, risks remain. Although AA and acetic acid is not as dangerous as acrolein, both have many health, safety and environmental risks associated with them. Firstly, at high concentrations and high temperatures, such as those for this process, AA and acetic acid form an explosive vapor. Exposure also causes irritation to the skin and eyes, and exposure for an hour or more can lead to injury or death. Despite this, the health

effects of AA and acetic acid are not as severe as acrolein (Sigma-Aldrich, 2019). Acrylic acid is also highly toxic in aquatic environments, however, does not accumulate in the environment as it is readily biodegradable (Arkema, 2012). Overall, AA and acetic acid do not pose as high a health and safety risk as acrolein, but many precautions must still be taken. As much of the risk from the manufacturing of AA is still present, DSN may deem that a total change in the process is not worth the incremental gain in safety.

Critical Review

One major assumption of both the FBR and PBR is that they have perfect mixing. However, for real-life scenarios, some areas of the reactor will have excellent mixing, whereas others would be 'dead zones'. PBRs are generally thought to have poorer mixing than FBRs, as they are susceptible to phenomena like channeling. However, if the superficial gas velocity within an FBR is not at a value ideal for fluidization, slugging may occur (Shih, 2019). Due to the highly turbulent flow within a fluidised bed, slugging is very difficult to predict. If slugging does occur, the gas bypass percentage would increase significantly, thus reducing the conversion rate and yield of AA.

Unequal mixing would also cause a greater reaction rate in the better mixed areas. This, in turn, will cause a temperature gradient across the reactor, with well mixed areas being especially hot, and dead zones being slightly colder. This also goes against the assumption that the FBR is isothermal. Furthermore, for the FBR, there will also be a significant temperature gradient along the height of the reactor, as the cooling fluid will heat up as it passes through the reactor. All these temperature gradients are exceptionally difficult to predict, due to the turbulent flow of the gas mixture.

An assumption unique to the PBR is that the cooling fluid temperature remains the same as it passes through the reactor, as the cooling fluid has a very large flowrate. However, there is incentive to keep the flowrate of the cooling fluid low, as this would save on OPEX. Furthermore, as the reactions taking place on the tube side of the reactor are highly exothermic, the cooling fluid in the shell is likely to experience some temperature difference. It is especially likely the cooling fluid that is close to the outer tube wall will be much hotter than the bulk cooling fluid. This issue can be alleviated by having better mixing on the shell side, perhaps by utilizing packing to induce more turbulent flow.

For the calculation of the superficial gas velocity, the ideal gas law was applied. This equation is most valid for gases at very low pressures, however the pressure within the reactor is reasonably high (over 2 bara), and the gas is extremely turbulent and constantly colliding with solid particles. For these reasons this assumption is not reasonable (Connor, 2019). Another issue with the calculation of superficial velocity is that the number of moles of gas changes through the reactor. All three reactions in Table 1 have fewer moles on the right side, and therefore the pressure will drop through the reactor. Determining an accurate value of the superficial gas velocity would require empirical data.

Another important assumption is that there are no impurities and only three reactions taking place. As the reactors operate at high temperatures, the likelihood of unwanted reactions taking place are high. The feed is also likely to contain many impurities, which are especially important to control in the propylene stream, as it is most likely to contain traces of other hydrocarbons (National Library of Medicine, 1994). Impurities and unwanted reactions will cause fouling on the catalyst, which will in turn reduce the reaction rate and yield of AA. Impurities and unwanted reactions will also cause fouling or damage to the reactor's internal components, which may reduce the efficiency of heat transfer from the cooling fluid to the reactants and catalyst.

When investigating how the FBR reacts to changes, it was found that temperature was the most sensitive variable. For example, when the operating temperature of the FBR was increased by just 10°C (to 312°C), the yield of acrylic acid fell below the 80% minimum requirement (to 78%). However, increasing temperature also decreased the area of heat transfer, and therefore lowered the shell diameter to below 4m (to 3.9m). DSN may want to consider sacrificing a high yield of acrylic acid for a smaller reactor diameter. As mentioned in the discussion section, as smaller diameter would allow existing plants to be retrofitted much more easily.

As the primary purpose of this exercise was to improve process safety, looking ahead, any possible safety failures should be investigated. For example, due to the highly exothermic nature of the reactions, a cooling system failure poses a huge risk, as the catalyst tends to coke-up at temperatures above 350°C and, more seriously, it may still be possible for a runaway reaction to occur. Any future investigation should aim to find how long the system can cope without cooling, as well as a consideration of what specifications a back-up cooling system would require.

Conclusions and Recommendations

In conclusion, the PBR seems to be the more appropriate reactor to use in this process instead of the FBR. This is because the PBR outperforms the FBR in several ways that cannot be overlooked. The first advantage of the PBR is that the dimensions are smaller, meaning the reactor will be easier to retrofit, as its dimensions are more like its predecessors. As seen in Table 3, the PBR covers a smaller area, due to its smaller shell diameter. Therefore, there will be more left-over space which can be filled with other equipment that could further improve the performance of the reactor. Also, as seen from Table 2, for the PBR, the yield for Acrylic Acid is higher, by around 8%, which reinforces the idea that the PBR is more efficient than the FBR. The total amount of Acrylic Acid produced in tonnes per year is also higher for the PBR by around 3800 tonnes per year, meaning the production of Acrylic Acid is more efficient within the PBR.

In both reactors, the inlet flowrates are very similar except the nitrogen feed, where the PBR N_2 feed is slightly higher, at 1500 kmol/hr. This would slightly increase the OPEX of the PBR. However, it must be remembered that the FBR also requires extra nitrogen to be added to the air inlet stream. The conversion values for propylene are also very similar for both reactors, and therefore there is no advantage for either option in this case.

In both cases, the Lower Flammability Limit of the mixture is lower than the Minimum Oxygen Concentration. Therefore, both reactors are safe and there is no risk of the adiabatic flame reaching the autoignition temperature, hence there is no risk of combustion within the reactor.

Despite this, the FBR uses less tubes to cool down the reaction, hence a lower CAPEX than the PBR. However, with all the other advantages the PBR possesses, it outweighs the small benefits that the FBR brings and therefore the PBR is still the best option to take when looking for a reactor for this process.

Recommendations

Both the FBR and PBR had a high conversion of propylene (89% and 88% respectively). However, over 10% of the propylene is still left over after the reaction, along with nitrogen and water. All these components can, and should, be recycled. Therefore, DSN may want to consider adding a recycling stream. Although this would significantly increase CAPEX and the plant footprint, it may reduce feedstock costs.

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Appendix

TABLE 6 lists the activation energies, pre-exponential factors and heat of reactions for the reactions

Reaction	E_i (kcal / kmol)	$k_{0,I}$ (kmol / (m^3 reactor h kPa^2))	ΔH_{RX} (kJ/mol)
1	15000	1.59×10^5	-590
2	20000	8.83×10^5	-1088
3	25000	1.81×10^8	-1926

TABLE 7 lists heat capacities for the fluids at reaction temperature

Propylene	AA	Acetic Acid	O_2	N_2	H_2O	CO_2
104.55	125.49	102.89	31.83	29.96	36.02	46.59

TABLE 8 lists the properties of the cooling fluid for the FBR.

Temperature in	200°C
Temperature out	250°C

Overall heat transfer coefficient	200 W / (m^2 K)	

TABLE 9 lists the upper and lower flammability limits (UFL and LFL respectively).

	Propylene	AA	Acetic Acid
LFL	2.0 vol%	2.4 vol%	4.0 vol%
UFL	11.1 vol%	8.0 vol%	19.9 vol%

$$-r_1 = k_1 \times e^{\left(\frac{-E_1}{RT}\right)} \times p_{propylene} \times p_{oxygen} \qquad \textit{Eq.20}$$

$$-r_2 = k_2 \times e^{\left(\frac{-E_2}{RT}\right)} \times p_{propylene} \times p_{oxygen} \qquad \textit{Eq.21}$$

$$-r_3 = k_3 \times e^{\left(\frac{-E_3}{RT}\right)} \times p_{propylene} \times p_{oxygen} \qquad \textit{Eq.22}$$

MATLAB Code

Fluidised Bed Reactor

```
%For a FBR (Fluidised Bed Reactor)


% R - Ideal Gas Constant in kJ/(kmol*K)
% Mr_[ ] - Relative molecuar mass of [ ] in kg/kmol
% p_total - Pressure of Reactor in kPa
% T_FBR - Temperature of Reactor in K
% Ea_[ ] - Activation Energy for reaction [ ] in kJ/kmol
% k0_[ ] - Pre-exponential constant of reaction [ ] in kmol/m^3
% DeltaH_[ ] - Enthalpy of reaction [ ] in kJ/mol
% F0_[ ] - Inital flowrate of [ ] in kmol/h
% F0( ) - Initial flowrate of [ ] in kmol/h (vector form, including gas
bypass)
% V0 - Initial reaction volume in m^3
% Vf - Final reaction volume in m^3
% F_[ ] - Flowrate of [ ] in kmol/h
% F_[ ]_fin - Final molar flowrate of [ ] in kmol/h
% Operating_time - Operating hours per year
% Product_[ ] - Acrylic acid produced per year in [ ]
% X_Propylene - Conversion of propylene
% Y_AA - Yeild of acrylic acid
% Q_[ ] - Energy released from reaction [ ] in kJ
% Q_FBR - Total Energy released from reactions in kJ
% U - Overall Heat Transfer Coefficient in kJ hr^-1 (m^2 * K)^-1
% T_cool_in - The temperature of cooling fluid going in to reactor in K
% T_cool_out - The temperature of cooling fluid going out of reactor in K
% LMTD - Log mean temperature difference in K
% A_ht - Area of Heat Transfer in m^2
% l - Height of reactor in m
% D0 - Outer diameter of cooling tubes in m
% l_cool - Total length of cooling tubes in m
% N_total - Number of cooling tubes
```

```matlab
% N_total_integer - Number of cooling tubes rounded up to nearest integer
% PR - Pitch ratio
% D_s - Diameter of reactor (derived from number of cooling tubes) in m
% D_l_ratio - Diameter to height ratio
% V_diff - Difference between Vf and derived reaction volume
% V_tot - Total reactor volume in m^3
% F_tot_initial_mol - Total initial molar flowrate (kmol/h)
% Vol_F_h - Volumetric flowrate of gas (m^3 / h)
% Vol_F_s - Volumetric flowrate of gas (m^3 / s)
% Sup_Vel - Superficial gas velocity (m / s)
% LFL_mix - Lower flamibility limit
% moc - Minimum oxygen concentration


% Clear variables and command window
clear
clc


% List global variables
global k0_1 k0_2 k0_3 Ea_1 Ea_2 Ea_3 R p_Total T_FBR y_Prop y_AA y_AC


% Universal gas constant
R = 8.314; % kJ/(kmol*K)


% Relative molecular mass
Mr_AA = 72.06; % kg/kmol
Mr_Prop = 42.08; % kg/kmol
Mr_O2 = 32; % kg/kmol
Mr_Water = 18; % kg/kmol


% The total pressure and the temperature chosen will be our
% operating conditions and will remain constant due the
% isothermal conditions within the PBR:


p_Total = (2*100); % kPa
T_FBR = 575; % K


% Constants for Reaction 1:


Ea_1 = 15000*4.184; % This is done to convert units from kcal/kmol to kJ/kmol
k0_1 = 1.59e+5; % kmol/m^3
DeltaH_1 = -590; % kJ/mol


% Constants for Reaction 2:
```

```matlab
Ea_2 = 20000*4.184; % This is done to convert units from kcal/kmol to kJ/kmol
k0_2 = 8.83e+5; % kmol/m^3
DeltaH_2 = -1088; % kJ/mol


% Constants for Reaction 3:


Ea_3 = 25000*4.184; % This is done to convert units from kcal/kmol to kJ/mol
k0_3 = 1.81e+8; % kmol/m^3
DeltaH_3 = -1926; % kJ/mol


% Initial Flowrates
F0_Prop = 100; % Initial flowrate of propylene (kmol/h)
F0_O2 = 222.8; % Initial flowrate of oxygen (kmol/h)
F0_Water = 180; % Initial flowrate of steam (kmol/h)
F0_N2 = F0_O2 / 21 * 79 + 500; % Initial flowrate of Nitrogen (kmol/h)


% Initial flowrates converted into vector form
% The 10 percent gas bypass must be considered


F0(1) = F0_Prop*0.9; % Initial flowrate of propylene, including gas bypass
(kmol/h)
F0(2) = F0_O2*0.9; % Initial flowrate of oxygen, including gas bypass (kmol/h)
F0(3) = 0; % Initial flowrate of acrylic acid (kmol/h)
F0(4) = 0; % Initial flowrate of acetic acid (kmol/h)
F0(5) = 0; % Initial flowrate of carbon dioxide (kmol/h)
F0(6) = F0_Water*0.9; % Initial flowrate of steam, including gas bypass
(kmol/h)
F0(7) = F0_N2*0.9; % Initial flowrate of nitrogen, including gas bypass
(kmol/h)


% The ODE's will be plotted against the reaction volume


V0 = 0; % m^3
Vf = 82; % m^3
space = 1000; % For linspace function
Vspan = linspace(0, Vf, space);


% From this, we can solve the ODE's


[V, F] = ode45(@FBR_Final, Vspan, F0);


% The flowrates of all components are listed in vector form
% The 10% gas bypass must be factored back in
```

```matlab
F_Prop = F(:,1) + (0.1*F0_Prop); % Flowrate of propylene across reactor in
kmol/h
F_O2 = F(:,2) + (0.1*F0_O2); % Flowrate of oxygen across reactor in kmol/h
F_AA = F(:,3); % Flowrate of acrylic acid across reactor in kmol/h
F_AC = F(:,4); % Flowrate of acetic acid across reactor in kmol/h
F_CO2 = F(:,5); % Flowrate of carbon dioxide across reactor in kmol/h
F_Water = F(:,6) + 0.1*F0_Water; % Flowrate of steam across reactor in kmol/h
F_N2 = F(:,7) + 0.1*F0_N2; % Flowrate of nitrogen across reactor in kmol/h


% Final molar flowrates (kmol / h)
F_AA_fin = F_AA(space,1); % Acrylic acid
F_O2_fin = F_O2(space,1); % Oxygen
F_Prop_fin = F_Prop(space,1); % Propylene
F_AC_fin = F_AC(space,1); % Acetic acid
F_CO2_fin = F_CO2(space,1); % Carbon dioxide
F_Water_fin = F_Water(space,1); % Water


% The mass of acrylic acid produced per year:


Operating_time = 8000; % h
Product_kmol = F_AA_fin*Operating_time; % AA produced in kmol/year
Product_kg = Mr_AA*Product_kmol; % AA produced in kg/year
Product_ton = Product_kg/1000; % AA produced in ton/year


Product_Disp = ['The FBR will produce ',num2str(Product_ton),' tonnes of
acrylic acid every year.'];
disp(Product_Disp)


% Plot dF against dV
plot (V, F_Prop, V, F_O2, V, F_AA, V, F_AC, V, F_CO2, V, F_Water)


title('Flowrates of components within the FBR');
xlabel('Reaction Volume (m^3)');
ylabel('Flowrate (kmol hr^(-1))');
legend({'Propylene','Oxygen','Acrylic Acid','Acetic Acid','Carbon
Dioxide','Water'});


% To calculate conversion of propylene:


X_Propylene = ((F0_Prop-F_Prop_fin)/F0_Prop);


X_Disp = ['The conversion of propylene is ',num2str(X_Propylene*100),'%'];
disp(X_Disp)
```

```matlab
%To find the yield of acrylic acid, we use the equation stated below:


Y_AA = F_AA_fin/(F0_Prop-F_Prop_fin);


Y_Disp = ['The yield of acrylic acid is ',num2str(Y_AA*100),'%'];
disp(Y_Disp)


% To calculate the heat transfer rate, the amount of heat transfer per product
would have to be calculated, hence, the total value will be our Q value:


Q_1 = F_AA_fin*(-DeltaH_1*1000); % kJ / h
Q_2 = F_AC_fin*(-DeltaH_2*1000); % kJ / h
Q_3 = (F0_Prop*X_Propylene - F_AA_fin - F_AC_fin) * (-DeltaH_3*1000); % kJ / h


% Note: The air inlet contains no traces of CO2


Q_FBR = Q_1 + Q_2 + Q_3; % kJ


U = 200 * 3.6; % kJ hr^-1 (m^2 * K)^-1
T_cool_in = 473.15; % K
T_cool_out = 523.15; % K


% Calculating the Log Mean Temperature Difference (LMTD) for a counter-current
heat exchanger:


dT1 = T_FBR - T_cool_out; % K
dT2 = T_FBR - T_cool_in; % K
LMTD = (dT1 - dT2)/log(dT1/dT2); % K


%The heat transfer area, can be calculated via:


A_ht = Q_FBR/(U*LMTD); %m^2


Aht_Disp = ['The heat transfer area for the FBR is ',num2str(A_ht),'m^2'];
disp(Aht_Disp)


%The diameter of the FBR can be calculated using the equation for area of
cylinder:


l = 7; % m
```

```matlab
l_Disp = ['The FBR height is ',num2str(l),'m'];
disp(l_Disp)


D0 = 0.0334; % m


l_cool = A_ht/(pi*D0); % m


% To calculate the total number of cooling tubes


N_total = l_cool/l;
N_total_integer = round(N_total + 0.5);


N_total_integer_Disp = ['The number of cooling tube required for the FBR is
',num2str(N_total_integer)];
disp(N_total_integer_Disp)


%The pitch ratio, is stated as 2.5;


PR = 2.5;


%Shell Diameter can be calculated via the equation below:


D_s = (2*(sqrt(N_total_integer/pi)) * PR * D0) + 2*D0; % m
D_s_Disp = ['The FBR diameter is ',num2str(D_s),'m'];
disp(D_s_Disp)


% Shell diameter to length ratio calculation:
D_L_ratio = l/D_s;
D_L_ratio_Disp = ['The diameter to length ratio of the FBR is
1:',num2str(D_L_ratio)];
disp(D_L_ratio_Disp)
% Difference between Vf and derived reaction volume (values should be similar)
V_diff = Vf - ((pi*(D_s/2)^2*l) - ((pi*(D0/2)^2)*l*N_total_integer));
V_diff_Disp = ['The difference between Vf and the derived reaction volume is
',num2str(V_diff), 'm^3'];
disp(V_diff_Disp)


% Calculation for total reactor volume
V_tot = pi/4*D_s^2*l; % m^3
V_tot_Disp = ['The total volume of the FBR is ',num2str(V_tot),'m^3'];
disp(V_tot_Disp)
```

```matlab
%Now to do the superficial gas velocity, assuming ideal gas:


F_tot_initial_mol = F0_Prop+F0_Water+F0_O2+F0_N2; % Total Initial molar
flowrate (kmol / h)
Vol_F_h = F_tot_initial_mol * R * T_FBR / p_Total; % Initial volumetric
flowrate (m^3 / h)
Vol_F_s = Vol_F_h / 3600; % Initial volumetric flowrate (m^3 / s)
Sup_Vel = Vol_F_s / ((pi*((D_s/2)^2))-(N_total_integer*pi*(D0/2)^2)); %
Superficial gas velocity (m / s)


Sup_Vel_Disp = ['The superficial gas velocity inside the FBR is
',num2str(Sup_Vel),'m/s.'];
disp(Sup_Vel_Disp)


%Lower flamability limit of the mixture:


LFL_mix = 1/((y_Prop/0.02) + (y_AA/0.024) + (y_AC/0.04));


%From this we can finally calculate the min. oxygen conc.:


moc = LFL_mix * (F0_Prop*4.5/F0_Prop);
moc_Disp = ['The minimum oxygen concentration of the FBR is ',num2str(moc)];
disp(moc_Disp)


if LFL_mix < moc
    disp('There is no risk of combustion in reactor')
elseif LFL_mix > moc
    disp('There is a risk of combustion in reactor')
end



function dFdV = FBR_Final(V,F)


global k0_1 k0_2 k0_3 Ea_1 Ea_2 Ea_3 R p_Total T_FBR y_Prop y_AA y_AC F_Total


F_Prop = F(1);
F_O2 = F(2);
F_AA = F(3);
F_AC = F(4);
F_CO2 = F(5);
F_Water = F(6);
F_N2 = F(7);
```

```matlab
%Partial Pressures of Propylene and Oxygen, the total flowrate is
%calculated first:


F_Total = F_Prop + F_O2 + F_AA + F_AC + F_CO2 + F_Water + F_N2;


%From this we can calculate the mole fraction of the Propylene and Oxygen


y_Prop = F_Prop/F_Total;
y_O2 = F_O2/F_Total;
y_AA = F_AA/F_Total;
y_AC = F_AC/F_Total;


%From this we can calculate the Partial Pressure of Propylene and O2


p_Prop = y_Prop*p_Total;
p_O2 = y_O2*p_Total;


%The reaction rate coefficients are also calculated to have an expression
%for the reaction rate:


k1 = k0_1*exp((-Ea_1/(R*T_FBR)));
k2 = k0_2*exp((-Ea_2/(R*T_FBR)));
k3 = k0_3*exp((-Ea_3/(R*T_FBR)));


%Defining the reaction rates:


r_1 = -k1*p_Prop*p_O2;
r_2 = -k2*p_Prop*p_O2;
r_3 = -k3*p_Prop*p_O2;


%Mole Balances


dFdV_Prop = r_1 + r_2 + r_3;
dFdV_O2 = ((3/2)*r_1) + ((5/2)*(r_2)) + ((9/2)*(r_3));
dFdV_AA = -r_1;
dFdV_AC = -r_2;
dFdV_CO2 =  -r_2 - (3*(r_3));
dFdV_Water = -r_1 - r_2 - (3*(r_3));
dFdV_N2 = 0;


dFdV(1) = dFdV_Prop;
dFdV(2) = dFdV_O2;
```

```
dFdV(3) = dFdV_AA;
dFdV(4) = dFdV_AC;
dFdV(5) = dFdV_CO2;
dFdV(6) = dFdV_Water;
dFdV(7) = dFdV_N2;


dFdV = dFdV';


end
```

Packed Bed Reactor

```
%For a PBR (Packed Bed Reactor)


% Cp_[ ] - Heat Capacity of [ ]
% R - Ideal Gas Constant
% Mr_[ ] - Relative molecuar mass of [ ]
% p_total - Pressure of Reactor
% T_FBR - Temperature of Reactor
% Ea_[ ] - Activation Energy for reaction [ ]
% k0_[ ] - Pre-exponential constant of reaction [ ]
% DeltaH_[ ] - Enthalpy of reaction [ ]
% F0_[ ] - Inital flowrate of [ ]
% V0 - Initial Volume
% Vf - Final Volume
% F_[ ] - Flowrate of [ ]
% Product_[ ] - Final flowrate of acrylic acid in [ ]
% X_Propylene - Conversion of propylene
% Y_AA - Yeild of acrylic acid
% Q_[ ] - Energy released from reaction [ ]
% Q_FBR - Total Energy released from reactions
% U - Heat Transfer Coefficient
% T_cool_in - The temperature of cooling fluid going in to reactor
% T_cool_out - The temperature of cooling fluid going out of reactor
% LMTD - Log mean temperature difference
% A_ht - Area of Heat Transfer
% l - Height of reactor
% D - Diameter of reactor (derived from volume and height)
% l_D_ratio - Height to diameter ratio
% D0 - Outer diameter of cooling tubes
% l_cool - Total length of cooling tubes
% N_total - Number of cooling tubes
% N_total_integer - Number of cooling tubes rounded up to nearest integer
% PR - Pitch ratio
% D_s - Diameter of reactor (derived from number of cooling tubes)
% D_diff - Difference between D and D_s
% Mavg - Average relative molecular mass of mixture
% dens_gas_in - density of gas inlet
% Vol_F_h - Volumetric flowrate of gas (m^3 per hour)
% Vol_F_s - Volumetric flowrate of gas (m^3 per second)
% Sup_Vel - Superficial gas velocity
```

```matlab
% LFL_mix - Lower flamibility limit
% moc - Minimum oxygen concentration


%Clear all variables and the command window
clear
clc


global k0_1 k0_2 k0_3 Ea_1 Ea_2 Ea_3 R p_Total T_PBR Cp_Prop Cp_O2 Cp_AA Cp_AC
Cp_CO2 Cp_Water U A_ht DeltaH_1 DeltaH_2 DeltaH_3 ...
  y_Prop y_O2 y_AA y_AC y_Water y_N2 F_Total


%The initial conditions and the constants given within the reactor


R = 8.314; % kJ/(kmol*K)
U = 200 * 3.6; %kJ hr^-1 (m^2 * K)^-1


Mr_AA = 72.06; %kg/kmol
Mr_Prop = 42.08; %kg/kmol
Mr_O2 = 32; %kg/kmol
Mr_N2 = 28; %kg/kmol
Mr_Water = 18; %kg/kmol


%The heat capacities of the components are given as:


Cp_Prop = 104.55; %J (mol K)^-1
Cp_O2 = 31.38; %J (mol K)^-1
Cp_AA = 125.49; %J (mol K)^-1
Cp_AC = 102.89; %J (mol K)^-1
Cp_CO2 = 46.59; %J (mol K)^-1
Cp_Water = 36.02; %J (mol K)^-1


%The total pressure and the temperature chosen will be our operating
%conditions and will remain constant due the isothermal conditions within
%the PBR:


p_Total = (2*100); %kPa
T_PBR = 528.15; %K


% Constants for Reaction 1


Ea_1 = 15000*4.184; % This is done to convert units from kcal/kmol to kJ/kmol
k0_1 = 1.59e+5; % kmol/m^3
DeltaH_1 = -590; % kJ/mol
```

```matlab
% Constants for Reaction 2


Ea_2 = 20000*4.184; %This is done to convert units from kcal/kmol to kJ/kmol
k0_2 = 8.83e+5; %kmol/m^3
DeltaH_2 = -1088; %kJ/mol


% Constants for Reaction 3


Ea_3 = 25000*4.184; %This is done to convert units from kcal/kmol to kJ/mol
k0_3 = 1.81e+8; %kmol/m^3
DeltaH_3 = -1926; %kJ/mol


%The ODE's will be plotted against the reaction volume


V0 = 0; % m^3
Vf = 18;% m^3
Vspan = linspace(0, Vf, 1000);


%The initial conditions for the balance equations are:


F0(1) = 100;  % Initial flowrate of Propylene (kmol/h)
F0(2) = 222.8; % Initial flowrate of Oxygen (kmol/h)
F0(3) = 0; % Initial flowrate of Acrylic Acid (kmol/h)
F0(4) = 0; % Initial flowrate of Acetic Acid (kmol/h)
F0(5) = 0; % Initial flowrate of Carbon Dioxide (kmol/h)
F0(6) = 180; % Initial flowrate of propylene (kmol/h)
F0(7) = 523.15; % Initial Temperature of the gas mixture (K)


F_N2 = 1500; % Flowrate of the inert Nitrogen gas into the reactor (kmol/hr)


%From this, we can solve the ODE's


[V, F] = ode45(@PBR_Final, Vspan, F0);


%To account for the 10% gas bypass, we add the 10% of our initial
%composition of gas to our final composition:


F_Prop = F(:,1); % Flowrate of Propylene across reactor in kmol/h
F_O2 = F(:,2); % Flowrate of Oxygen across reactor in kmol/h
F_AA = F(:,3); % Flowrate of Acrylic Acid across reactor in kmol/h
```

```matlab
F_AC = F(:,4); % Flowrate of Acetic Acid across reactor in kmol/h
F_CO2 = F(:,5); % Flowrate of Carbon Dioxide across reactor in kmol/h
F_Water = F(:,6); % Flowrate of Water across reactor in kmol/h
T = F(:,7); % Temperature change across reactor in K


Product_kmol = F_AA(1000,1)*8000;
Product_kg = Mr_AA*Product_kmol; % Total amount of Acrylic Acid Produced in kg
/ yr
Product_ton = Product_kg/1000; % Total amount of Acrylic Acid Produced in
Tonnes / yr


% Display amount of acrylic acid produced per year
Product_Disp = ['The PBR will produce ',num2str(Product_ton),' tonnes of
acrylic acid every year.'];
disp(Product_Disp)


%Graphs for the respective flowrates of the components


plot (V, F_Prop, V, F_O2, V, F_AA, V, F_AC, V, F_CO2, V, F_Water)


title('Flowrates of components within the PBR');
xlabel('Reaction Volume (m^3)');
ylabel('Flowrate (kmol hr^(-1))');
legend({'Propylene','Oxygen','Acrylic Acid','Acetic Acid','Carbon
Dioxide','Water'},'Location','east');


%Graph for the temperature change across the reactor


plot(V, T)


title('Temperature change in the PBR');
xlabel('Reaction Volume (m^3)');
ylabel('Temperature (K)');


%Conversion of Propylene


X_Propylene = ((F0(1)-F_Prop)/F0(1));
X_Propylene(1000,1);
X_Disp = ['The conversion of propylene is
',num2str(X_Propylene(1000,1)*100),'%'];
disp(X_Disp)


%To find the yield, we use the equation stated below:
```

```matlab
Y_AA = F_AA/(F0(1)-F_Prop);
Y_AA(1000,1000);
Y_AA_Disp = ['The yield of Acrylic Acid is
',num2str(Y_AA(1000,1000)*100),'%'];
disp(Y_AA_Disp)


%To calculate the heat transfer rate, the amount of heat transfer per product
%would have to be calculated, hence, the total value will be our Q value:
%Note: The air inlet contains no traces of CO2


Q_AA = F_AA*(-DeltaH_1*1000); %kj / hr
Q_AC = F_AC*(-DeltaH_2*1000); %kj / hr
Q_CO2 = (F_CO2/3) * (-DeltaH_3*1000); %kj / hr


Q_FBR = Q_AA + Q_AC + Q_CO2;


%Our overall heat tarnsfer coefficient and inlet and outlet for the cooling
%fluid will be stated before the calculation of the heat transfer area:


U = 200 * 3.6; %kJ hr^-1 (m^2 * K)^-1
T_cool_in = 473.15; %K
T_cool_out = 523.15; %K


%Calculating the Log Mean Temperature Difference (LMTD) for a
%counter-current heat exchanger:


dT1 = T_PBR - T_cool_out; %K
dT2 = T_PBR - T_cool_in; %K
LMTD = (dT1 - dT2)/log(dT1/dT2); %K


%The heat transfer area, can be calculated via:


A_ht = Q_FBR/(U*LMTD); %m^2
A_ht(1000,1);
Aht_Disp = ['The heat transfer area for the PBR is
',num2str(A_ht(1000,1)),'m^2'];
disp(Aht_Disp)


%The diameter of the FBR can therefore be calculated using basic equation of
%area of cylinder:
```

```matlab
l = 5; %m
l_Disp = ['The PBR height is ',num2str(l),'m'];
disp(l_Disp)


D = ((4*Vf)/(l*pi))^(1/2); %m
D_Disp = ['The PBR diameter is ',num2str(D),'m'];
disp(D_Disp)


D_L_ratio = l/D;
D_L_ratio_Disp = ['The diameter to length ratio of the PBR is
1',num2str(D_L_ratio)];
disp(D_L_ratio_Disp)


%The pitch ratio, is stated as 1.5;


PR = 1.5;


%To find the value of the length of cooling tube:


Di = 0.02; %m
l_cool = A_ht/(pi*Di); %m


%To calculate the total number of cooling tubes, we use N_total = l_cool/l,
which gave us the number to cooling tubes, which is
%rounded up to the nearest integer


N_total = l_cool/l;
N_total(1000,1);
N_total_integer = round(N_total(1000,1) + 0.5);


N_total_integer_Disp = ['The number of cooling tube required for the PBR is
',num2str(N_total_integer)];
disp(N_total_integer_Disp)


%Shell Diameter can be calculated via the equation below:


D_s = (2*(sqrt(N_total_integer/pi)) * PR * Di) + 2*Di; %m
D_s_Disp = ['The shell diameter for the reactor is ',num2str(D_s), 'm'];
disp(D_s_Disp)


%The volume of the reactor will then be given as:
```

```matlab
V_reactor = (pi*(D_s/2)^2)*l;
V_reactor_Disp = ['The volume of the reactor is ',num2str(V_reactor), 'm^3'];
disp(V_reactor_Disp)


%Now to do the superficial gas velocity, assuming ideal gas:


Vol_F_h = (F_Total * ((R*T_PBR)/p_Total)); % m^3 / h
Vol_F_s = Vol_F_h / 3600; % m^3 / s
Sup_Vel = Vol_F_s / (N_total_integer*(pi*((Di/2)^2))); %m / s


Sup_Vel_Disp = ['The superficial gas velocity inside the PBR is
',num2str(Sup_Vel),'m/s.'];
disp(Sup_Vel_Disp)


%Lower flamability limit of the mixture:


LFL_mix = 1/((y_Prop/0.02) + (y_AA/0.024) + (y_AC/0.04))


%From this we can finally calculate the min. oxygen conc.:


moc = LFL_mix * (F0(2)/F0(1))


if LFL_mix < moc
    disp('There is no risk of combustion in reactor')
elseif LFL_mix > moc
    disp('There is a risk of combustion in reactor')
end


V_tubes_total = (pi*(Di/2)^2)*l*N_total_integer
Vf



function dFdV = PBR_Final(V,F);


global p_Prop p_O2 k0_1 k0_2 k0_3 Ea_1 Ea_2 Ea_3 R p_Total T_PBR y_Prop y_O2
y_AA y_AC y_Water y_N2 F_Total


F_Prop = F(1);
F_O2 = F(2);
F_AA = F(3);
F_AC = F(4);
F_CO2 = F(5);
F_Water = F(6);
```

```matlab
T = F(7);


%The inert gas that will be used is Nitrogen, will have a constant flowrate
%in the packed bed reactor:


F_N2 = 1500;


%Partial Pressures of Propylene and Oxygen, the total flowrate is
%calculated first:


F_Total = F_Prop + F_O2 + F_AA + F_AC + F_CO2 + F_Water + F_N2;


%From this we can calculate the mole fraction of the components


y_Prop = F_Prop/F_Total;
y_O2 = F_O2/F_Total;
y_AA = F_AA/F_Total;
y_AC = F_AC/F_Total;
y_Water = F_Water/F_Total;
y_N2 = F_N2/F_Total;


%From this we can calculate the Partial Pressure of Propylene and O2


p_Prop = y_Prop*p_Total;
p_O2 = y_O2*p_Total;


DeltaH_1 = -590;
DeltaH_2 = -1088;
DeltaH_3 = -1926;%


U = 200 * 3.6;
A_ht = 1.137e3;


Cp_Prop = 104.55; %J (mol K)^-1
Cp_O2 = 31.38; %J (mol K)^-1
Cp_AA = 125.49; %J (mol K)^-1
Cp_AC = 102.89; %J (mol K)^-1
Cp_CO2 = 46.59; %J (mol K)^-1
Cp_Water = 36.02; %J (mol K)^-1


%The reaction rate coefficients are also calculated to have an expression
%for the reaction rate:
```

```matlab
k1 = k0_1*exp((-Ea_1/(R*T_PBR)));
k2 = k0_2*exp((-Ea_2/(R*T_PBR)));
k3 = k0_3*exp((-Ea_3/(R*T_PBR)));


%Defining the reaction rates:


r_1 = -k1*p_Prop*p_O2;
r_2 = -k2*p_Prop*p_O2;
r_3 = -k3*p_Prop*p_O2;


%Mole Balances:


dFdV_Prop = r_1 + r_2 + r_3;
dFdV_O2 = ((3/2)*r_1) + ((5/2)*(r_2)) + ((9/2)*(r_3));
dFdV_AA = -r_1;
dFdV_AC = -r_2;
dFdV_CO2 =  -r_2 - ((1/3)*(r_3));
dFdV_Water = -r_1 - r_2 - (3*(r_3));


%Energy Balance:


dTdV = (((r_1*DeltaH_1*1000) + (r_2*DeltaH_2*1000) + (r_3*DeltaH_3*1000)) ...
    - (U*A_ht*(F(7) -
T_PBR)))/((F(1)*Cp_Prop)+(F(2)*Cp_O2)+(F(3)*Cp_AA)+(F(4)*Cp_AC)+(F(5)*Cp_CO2)+
(F(6)*Cp_Water));


dFdV(1) = dFdV_Prop;
dFdV(2) = dFdV_O2;
dFdV(3) = dFdV_AA;
dFdV(4) = dFdV_AC;
dFdV(5) = dFdV_CO2;
dFdV(6) = dFdV_Water;
dFdV(7) = dTdV;


dFdV = dFdV';


end
```