

The reactor design project engineering essay



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The project objective was to optimize three different adiabatic ammonia reactor configurations with respect to reactor performance in order to produce 800 tonnes of ammonia per day, or the molar equivalent of 0.5447 kmol s⁻¹ of ammonia. The optimizations in reactor performance involved primarily, minimizing the catalyst volume and secondarily, maximizing the catalyst lifespan, as well as ensuring the final operating conditions were stable. Due to the absence of a cost function, the reactor could NOT be optimized with respect to cost minimization.

Three different reactor types were considered, namely a single plug-flow reactor, a dual interstage cooling reactor and a dual cold-shot cooling reactor. Temperature, pressure and fraction of ammonia in the feed stream were found to have the greatest effect on the resultant catalyst volume. Using MATLAB, it was found that the minimum volumes were 9.61 m³, 3.94 m³ and 4.78 m³ for a single stage plug-flow, an interstage cooling configuration and a cold shot cooling reactor configuration respectively. The interstage cooling reactor allowed for a 59% decrease in total catalyst volume when modified from the single stage design, but required an increase in inlet feed temperature of 115K and 2 additional heat exchangers. The cold shot cooling method allowed for a 50.2% decrease in reactor volume from the single stage design, requiring a 75K increase in feed temperature.

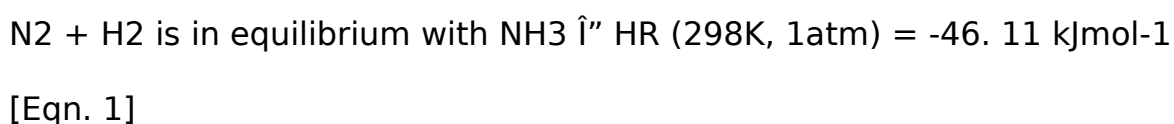
1. Introduction

1.1. Background

Ammonia synthesis (also known as the Haber process) is one of the most widely applied chemical processes in the world; in 2009, the total worldwide

production of ammonia exceeded 133,000 metric tonnes, this is second only to the worldwide production of sulphuric acid. Most of the ammonia produced is used in the manufacture of fertilisers (such as ammonium nitrate), ammonia is also used in the manufacture of nitrogen-based polymers such as nylon. Another noteworthy use of ammonia is as the starting reagent for the manufacture of nitrogen-based explosives such as nitroglycerin.

The reaction which generates ammonia is exothermic and equilibrium limited:



In the early 20th century, Fritz Haber discovered that in order to obtain a significant yield of ammonia, the reaction required both high pressures and low temperatures (in accordance with the van 't Hoff-Le Chatelier principle). It was known that the rate at which N_2 decomposed in the reaction was very slow (N_2 is thermodynamically more stable than NH_3); therefore a very efficient catalyst was required in order to facilitate ammonia formation. Nowadays, the catalyst used in most industrial ammonia reactors is usually a porous form of enriched iron. Catalysts are expensive, but they present a good trade off; reactors are able to produce sufficient amounts of product at lower, more manageable temperatures and pressures.

1.2. Design objective

The overall objective was to design a continuous fixed bed plug-flow process to meet the company's daily ammonia production demand of 800 tonnes per

day (exclusive of any ammonia in the feed). The primary design objective was to try to minimize the catalyst volume the process required in order to meet the production requirement. The design also had to be considered safe to operate and had to operate at conditions that were considered to maximize the lifespan of the catalyst; these two were considered as secondary objectives. The preliminary design of the reactor considered a single-stage adiabatic bed with a bed cross-sectional area of 2.0 m². The final designs involved two different two-stage systems; one implementing interstage cooling and the other implementing cold-shot cooling.

Reactor performance and sensitivity were analysed by observing the effects of altering specific operating and design variables. The cost function for the process was not known, therefore it is important to note that the reactor could not be 'optimized' with respect to cost, however the design could be implemented such that the reactor performance was greatly improved. For example, minimizing the required catalyst volume (and hence minimizing the reactor volume) will reduce the construction cost of the reactor. However this may come at the expense of greater operating and maintenance costs and, in the case of two-stage systems, may result in additional construction costs (interstage cooling requires heat exchanger(s) to be built). The investigation will only allow qualitative suggestions to be made as to which specific design aspects contribute to the generation and/or reduction of costs.

1.3 Safety

The reactor operating conditions should be stable; such that small disturbances will not lead to thermal runaway (which has important

implications for safety). Other than that, there are no large risks involved with operating the ammonia reactor, provided that good process control is implemented by the operator.

2. Kinetic theory and types of reactor configurations

2. 1. The kinetics of ammonia synthesis and its implications on reactor design

Ammonia synthesis involves a single exothermic, reversible reaction between nitrogen and hydrogen. For reversible reactions, the conversion corresponding to thermodynamic equilibrium at the chosen operating conditions cannot be surpassed. Since the reaction is exothermic, the activation energy (which is only temperature dependent) of the backwards reaction is greater than that of the forward reaction. Therefore an increase in temperature causes a rise in the rate of the reverse reaction which is greater than the rise in the rate of the forward reaction thus decreasing the maximum attainable conversion but decreasing the required catalyst volume. On the other hand, operating at a lower temperature increases the maximum attainable conversion, whilst reducing the total reaction rate and increasing the required catalyst volume. With regard to pressure, the effect is the opposite; increasing the pressure causes a greater rise in the rate of the forward reaction compared the backward reaction and vice versa.

Designing a reactor producing ammonia therefore requires a compromise between keeping temperatures sufficiently high such that reaction rate remains significant whilst obtaining a respectable conversion of ammonia. Similarly, the pressure should be great enough so as to maintain a significant

reaction rate, but not so high as to cause the reactor to deviate from safe operation.

In order to minimize catalyst volume (and meet the primary objective), it is desirable to operate at the maximum forward rate of reaction at each cross-section across the reactor; thus maximizing the average forward rate across the reactor, this allows the desired extent to be met with the minimum catalyst surface area and hence with the minimum catalyst volume. In order for this to occur, each cross-section in the reactor must be operated at the unique pressure and temperature required to achieve maximum rate for a particular extent, i. e. the reactor moves along the locus of maximum reaction rates. This is unfeasible in this investigation since there is no temperature or pressure control implemented across the reactor (the reactor is adiabatic and $W_{SHAFT} = 0$); and even so, maintaining specific pressures and temperatures at each point along the reactor is practically unfeasible in itself; as each point in the reactor would require its own heat exchanger and pressure control system.

Therefore for exothermic reversible reactions (without heat removal), the temperature increases along the length of the reactor and the rate vs extent profile will always have a characteristic maximum because the temperature along the reactor increases due to the heat released by the reaction, causing the net production rate to increase up to a certain extent before the reverse reaction starts to become significant. As the rate of the backwards reaction tends to increase further and temperature rises, the overall reaction rate will eventually reach zero at equilibrium.

2. 2. Brief description of the Plug-Flow Reactor (PFR)

A plug-flow reactor is characterized by fluid flowing through one end of the reactor and out the other, whilst satisfying the assumptions of plug-flow. The assumptions state:

Fluid properties and flow rate remain constant across any cross-section of the reactor.

The flow is orderly, with no element overtaking or mixing with fluid ahead or behind, (i. e. the residence time is the same for all fluid elements).

The above assumptions tend to hold true where there is turbulent flow ($Re > 105$), ensuring good radial mixing, and if the ratio of reactor length to diameter of the reactor is large (ratio $\hat{\%} \approx 50$), where lateral mixing may be neglected 2.

Figure 1: An illustration of a plug-flow reactor 3

2. 3. Brief description of Interstage Cooling

Interstage cooling, also known as intercooling, is a multiple reactor design suitable for exothermic reversible reactions. Heat exchangers are used to cool the output of each reactor before being passed on to the next reactor, allowing for a greater possible conversion to be achieved in each successive reactor. This process can be replicated for an indefinite number of reactors until the reactor temperature is too low for reactions to occur or until the decrease in catalyst volume is not worth the additional cost of construction and complexity of operation. This project considers only the case where two reactors are used.

Figure 2: An illustration of a dual reactor interstage cooling system⁴

2. 4. Brief description of Cold-shot Cooling

Cold-shot cooling reactor designs are similar to that of interstage cooling, but allow for elimination of the intermediate heat exchangers by injecting cold feed directly into the outlets of each reactor. This addition cools down the outlet stream of the reactor and also has the effect of decreasing the composition and conversion of the flow into the subsequent reactor (corresponding to the path from point 'b' to 'c' in Figure 3 below).

Figure 3: An illustration of a dual reactor cold-shot cooling system ⁵

The flow diagram of two cold-shot reactors illustrates the lack of heat exchangers as compared to interstage cooling, as well as the splitting of the initial feed stream by the splitting fraction α , \hat{I}_{\pm} , which is the fraction of the fresh feed used as the coolant. The extent of reaction remains constant after mixing (which can be proven by a mass balance).

3. Mathematical model - Derivations of differential equations

All the assumptions of plug-flow mentioned above were applied in the construction of the equations below; the reactor was also assumed to operate at steady state (there is no mass hold up due to the catalyst). All other assumptions are mentioned in the derivations. It should be noted that r_{NH_3} is defined as (r_{NH_3} generated - r_{NH_3} consumed) and is measured per unit of catalyst volume; hence the equations specify the volume of catalyst V_C and not the reactor volume V_R .

3. 1. Change in catalyst volume with respect to the extent of reaction:

Mass balance on ammonia: [Eqn. 2]

The extent of reaction can be defined as:

[Eqn. 3]

Equations 2 and 3 were combined to obtain the following equation:

Since , the equation above was rearranged to give the initial catalyst volume gradient:

[Eqn. 4]

3. 3. Change in temperature with respect to the extent of reaction:

Figure 4: An illustration of the cross section of a plug-flow reactor

An energy balance across an infinitesimally small cross section of the catalyst bed gave:

Shaft work (W), changes in kinetic energy and changes in potential energy were neglected:

The equation above was divided by the cross-sectional area of the tube, A :

where Q denotes the heat transfer by conduction.

In the equation below, the enthalpy change upon mixing was neglected (a perfect solution was assumed). It was also assumed that the gases in

question were ideal and hence their enthalpy was independent of pressure, the energy balance then took the form:

[Eqn. 5]

is the standard heat of formation of compound.

'i' denotes each species present.

Recalling that for a tubular reactor, and :

does not have a negative sign as r_{product} is calculated as the main subject)

[Eqn. 6]

The heat of reaction was simplified as shown below:

[Eqn. 7]

Equation 7 was substituted into Equation 6 which was then substituted into Equation 5:

[Eqn. 8]

The chain rule was used to combine and :

Since the reactor was assumed to be adiabatic, $Q = 0$:

[Eqn. 9]

3. 4. Change in pressure with respect to the extent of reaction:

The chain rule was used to find using the formula for , bed cross-sectional area A and since $A dl = dVC$.

Substituting the components of the three terms above, we get the initial pressure against extent gradient formula:

[Eqn. 10]

4. Simulation - theory and strategy

4. 1. Main simulation objectives

Regardless of the design used, these objectives are overarching and apply to all three reactor types: The first two bullet-points define what is meant by optimizing the reactor:

Minimizing catalyst volume;

Operating temperatures and pressures are limited by safety considerations (preventing thermal runaway), material construction and catalyst degradation conditions. These degradation conditions are specified by actual limits set by ammonia process operators in industry: these are above 823 K and above 300 bar 6;

Interstage and cold-shot cooling designs are only dual reactor designs.

The derivation of the required total extent for all simulations is as follows:

The MATLAB coding incorporating the required data and was used to solve the differential equations described earlier in the mathematical model for the
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outlet temperature, pressure and catalyst volume; all the assumptions applied in the mathematical model were thus applied in the coding, unit consistency was also maintained in the programming.

4. 2. Single stage simulation strategy

It is clear that a plug-flow reactor can take advantage of concentration profiles present in the reactor in order to minimize the total catalyst volume. Near the desired extent, adiabatic plug-flow reactors (running exothermic reversible reactions) operate ideally somewhere between the equilibrium line, where the rate of the forward and backwards reaction are equal, and the optimum line, which is a curve connecting the maximas of all the different rate curves, also known as the locus of maximum rates.

Figure 5: A graph displaying the variation of forward rate with extent It is opted to run the reactor under conditions such that the inlet rate is exactly equal to the outlet rate where the reactor exits at the desired extent of 0.5447. The " $r_{in} = r_{out}$ " condition limits the maximum average rate by a small amount but provides a greater amount of kinetic stability in the event of a disturbance; a small increase in the inlet temperature may push the reaction closer to equilibrium whilst a small decrease in the inlet temperature will decrease the outlet rate slightly but still allow the reactor to operate in a region of higher rates. The locus of " $r_{in} = r_{out}$ " is found between the optimum line and the equilibrium line.

As shown in Figure 5, this condition also means that the region of maximum reaction rate is taken advantage of; i. e. the rate in the reactor is always

greater than or equal to the inlet rate. Therefore, although the temperature increases along the reactor, the forward rate is kept as high as possible.

As the extent of reaction increases across the reactor for a fixed set of inlet conditions, it is expected for the surface area of catalyst to increase; if more product is generated, more catalyst is required to facilitate this generation. There is a limit in the MATLAB coding such that the catalyst volume decreases whilst the reaction extent continues to increase; the code is such that results after this point are treated as erroneous and are not used, thus the code finds the inlet conditions needed to achieve the maximum possible extent for an adiabatic reactor.

To apply the simulation strategy, a MATLAB program was created to find the inlet conditions which satisfy the " $r_{in} = r_{out}$ " condition for a desired final extent (0.5447 in this case). A separate program was also created to vary operating and design conditions individually and examine their effect on the catalyst volume. Graphs of the locus of maximum reaction rate, locus of " $r_{in} = r_{out}$ " rates and the equilibrium curve were constructed using the desired inlet conditions determined from the single stage simulation.

4. 3. Interstage cooling simulation strategy

The overall reaction follows the adiabatic operating curve (it may not necessarily be a straight line due to the pressure drop across the reactor). It was desirable for the reaction to end at the same point as in the single stage simulation (with the same final extent); where the rate at the outlet of the second reactor lies on the " $r_{in} = r_{out}$ " line for the desired extent. It was also desirable for the rate at the exit of the first reactor to be equal to the rate at

the entrance of the second reactor; so that the reactor can continue onwards from the same rate in the second reactor (and maintain the average forward reaction rate).

For this code, there was no condition that the rate at the inlet of the first reactor must equal the rate at the outlet of the first reactor (and likewise for the second reactor); since it was unfeasible to make the rates equivalent at all the inlets and outlets. Instead it was specified that $\text{rate1 OUT} = \text{rate2 IN}$ and that $\text{rate2 OUT} = \text{rate OPTIMIZED SINGLE STAGE OUT}$.

The extent in the first reactor (and therefore in the second reactor) had to be specified for each set of results. If the extent was too high, the outlet of the first reactor would be very near equilibrium whilst if it was set too low the outlet of the first reactor would be reached before the maximum rate had been obtained; therefore a degree of overshoot past the maximum reaction rate was desirable; the program ensured that there was a degree of overshoot past the maximum reaction rate in both reactors before validating a result.

The locus of maximum reaction rates (from the single stage optimization) was used to determine the feed temperature for which the rate is a maximum at the start; this temperature was roughly 790K (located graphically). Above this temperature, the region of maximum reaction rates was not utilised at all; and the maximum extent achievable (using the gradient of the operating line) at equilibrium was roughly 0.28. This specified the minimum extent of reaction in reactor 1. If the feed temperature were too low, the first reactor would perform similar to a single

PFR, defeating the purpose of having two reactors. Thus a moderate extent range of 0.3 - 0.4 was chosen for the first reactor as it was unworkable to put an excessive production load on either reactor.

In order to apply this strategy, a program was used to specify the inlet conditions to the second reactor; the program moved along the operating curve using the initial conditions obtained in the single stage reactor up to the desired extent in the first reactor. This gave the inlet rate to the second reactor as well as the flow rate, temperature and composition of this stream. Following this, the $\text{rate1 OUT} = \text{rate2 IN}$ condition was used to acquire the inlet and outlet temperatures and pressures of the first reactor and its volume. Lastly, the inlet conditions to the second reactor and the remaining extent were used to calculate the volume of the second reactor. The combined volumes and degrees of cooling between the reactors were compared for the chosen range of extents.

4. 4. Cold-shot cooling simulation strategy

Figure 6: A graph displaying the variation of extent with temperature for a cold-shot system

The rate identity " $r_{in} = r_{out}$ " used to optimize the single PFR was used in the cold-shot cooling reactor design. With reference to Figure 6, optimization was achieved by ensuring that the reaction moved from points a f c d , with the following rate identities; $r_a = r_b$ and $r_e = r_d$. The second reactor would operate along the path that the optimum single PFR would operate on (e f d).

By adhering to the above conditions, there were three variables left to define, namely alpha ($\hat{\alpha}$), initial feed temperature T_{in} and the interstage extent \hat{X}_1 . Fixing alpha and T_{in} would automatically define \hat{X}_1 and outlet temperature of the first reactor as the rates at points 'a' and 'b' must be the same. This optimized the first reactor for the given inlet conditions. By constructing enthalpy and mass balances on the mixing point of the outlet from the first reactor with the cold stream, the inlet temperature into the second reactor was determined, thereby finding outlet conditions of the second reactor, should it achieve the required extent of 0.5447 kmol s⁻¹. Finally, in order to ensure that total optimization had occurred for the specified alpha and temperature, the difference in rates at points 'e' and 'd' was confirmed to be as close to zero as possible. Several iterations would be required to home in on the best inlet temperature for a given extent.

The temperature of the feed used for cooling, T_f , was 298K; significantly lower than the temperature of the fluid exiting the reactor. This imposed an upper limit on the split fraction $\hat{\alpha}$, beyond which the feed temperature into the second reactor would be too low for reactions to operate at an acceptable rate; catalyst volume would need to be larger to counter this effect, meaning optimization would not be achieved.

Therefore, by varying $\hat{\alpha}$ for 50 equal intervals from 0.01 to 0.5, and finding the 50 corresponding T_{in} values that satisfied the above stated rate identities gave the optimum reactor for each value of $\hat{\alpha}$. The best cold-shot reactor specification was easily deduced from the setup which had the smallest overall catalyst volume.

Results and Discussion

5. 1. Single Plug-flow Reactor

5. 1. 1. Varying the ammonia composition in the feed

Figure 7: A graph displaying the effect of ammonia feed mol % change on catalyst volume

The composition of ammonia in the feed was changed while keeping the molar feed rate constant. (Change ratio: 4% decrease in NH_3 = 1% increase in N_2 + 3% increase in H_2 , etc).

Figure 7 shows that decreasing the ammonia fraction from the original 8 mol % (while increasing the reactant mol %) lead to a significant drop in catalyst volume required. The greater concentration of reactants favoured the forward reaction, increasing the rate of formation of ammonia, leading to a smaller catalyst volume. When the ammonia fraction was too high ($\hat{\alpha}\% \approx 0.16$), the initial concentration of reactants was insufficient to achieve the required extent. Also, as the partial pressure of ammonia increased in the reactor, a greater proportion of the catalyst's active sites became blocked and the forward rate decreased, increasing the required catalyst volume 7.

It was decided to keep the mol % of ammonia in the feed at 8% in subsequent simulations; although the lowest mol % of ammonia in the feed produces the minimum catalyst volume, it is impractical for this to occur since ammonia is normally recycled in industrial reactors 8.

5. 1. 2. Varying the reactor cross-sectional area

Figure 8: A graph displaying the effect of cross-sectional area on catalyst volume

Figure 8 shows that increasing the cross-sectional area reduced the catalyst volume, but this reduction was more significant only at the smaller area values. Increasing the area increased the number of catalyst pellets available at the reactor cross-section; therefore a greater reaction rate was initially facilitated as the volume increased. However, the inlet flow was fixed, and beyond a certain area, the flow into the reactor did not utilise the additional pellet area at the cross section; and thus the catalyst volume was less affected. The cross sectional area for the remainder of the investigation was kept at 2m² because the increase in cross-sectional area above 2m² does not justify the relatively minimal reduction in catalyst volume.

5. 1. 3. Variation of catalyst voidage

Table 1: Displays catalyst volumes for different values of catalyst voidage

Voidage

0. 7

0. 6

0. 5

0. 4

0. 3

V_c at $\hat{I}^{3/4} = 0.54466$ (m³)

23.4642

23.4877

23.5399

23.6728

24.1043

Voidage is the ratio of the catalyst volume to the reactor volume. A larger voidage means a higher catalyst pellet density, thereby allowing a smaller catalyst volume. However, increases in voidage past 0.4 did not contribute to any further significant decrease in catalyst volume. For the purpose of subsequent simulations, the voidage was kept to the original 0.4.

5.1.4. Variation of catalyst diameter

Table 2: Displays catalyst volumes for different values of catalyst diameter

Catalyst Diameter

0.011

0.009

0.007

0.005

0.003

V_c at $\hat{I}^{3/4} = 0.54466$ (m³)

23.5881

23. 6209

23. 6728

23. 7675

23. 9954

It is seen from the data that varying catalyst diameter had a negligible effect on the catalyst volume, suggesting that although the surface area of each catalyst pellet increased, the number of catalyst pellets decreased, and thus the overall catalyst area did not change significantly. It was decided to stick to the original catalyst diameter provided.

5. 1. 5. Varying temperature and pressure

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Figure 8: A graph displaying the effect of inlet temperature on catalyst volume for different isobars

As the temperature was increased, a decrease in the catalyst volume was observed. At lower pressures, the gradient of the graph (the change in VC with inlet T) was much higher and therefore inlet temperature was more effective at reducing the catalyst volume at lower pressures. This has some implications with respect to cost; if the inlet temperature is increased, there is an electricity cost associated with operating the reactor at this higher inlet temperature, but there is also a saving due to the reduction in catalyst volume.

Figure 9: A graph displaying the effect of inlet pressure on catalyst volume for different isotherms

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As inlet pressure was increased, the catalyst volume decreased. As discussed in the theory, the increase in pressure favoured the forward reaction, thereby increasing the reaction rate per unit volume of catalyst. However, the capital costs spent on reactor materials able to withstand the high pressures have to be taken into consideration in addition to the greater maintenance cost of the catalyst bed (since a higher pressure reduces the longevity of a catalyst).

5. 1. 6. Results of single stage simulation

Table 3: Displays the specifications and feed conditions the optimized single PFR

Feed Composition

Cross

sectional area

(m²)

Catalyst Diameter

(m)

Voidage

Extent

Temperature

(K)

Pressure

(Bar)

N₂

H₂

NH₃

In

Out

In

Out

0.23

0.69

0.08

2

0.0007

0.4

0.5447

624.2

796.0

300

298.6

It can be observed that the pressure drop throughout the reaction was rather insignificant compared to the total pressure in the reactor. The optimization values from the single stage plug-flow reactor were essential for designing dual reactors that utilized interstage or cold-shot cooling as the second reactors were designed to follow the reaction path taken by the single stage PFR.

The optimum single stage pressure of 300 bar was also the optimum pressure used for the subsequent simulations; the maximum operating pressure tolerable is 300 bar according to the catalyst degradation conditions specified in the simulation objectives.

5. 2. Interstage Cooling

Figure 10: A graph displaying the extents of reaction for different temperatures. The interstage path for \hat{V}_1 values of 0. 3, 0. 34 (optimum), and 0. 4 are displayed along with the locus of maximum reaction rates, the equilibrium curve and the locus of $r_{in} = r_{out}$.

Results were obtained for 10 extents between 0. 3 and 0. 4; these are displayed in the appendix. From the graph above, it can be seen that for all three extents; 0. 3, 0. 34, 0. 4, the reaction in the first reactor moved past the locus of maximum rates and the locus of " $r_{IN} = r_{OUT}$ " and then approached the equilibrium curve, thereby maximizing conversion. The outlet stream was then cooled to a point along the path taken by the volume minimizing single PFR. The graph thus shows that performance optimization occurred in the interstage cooling design as catalyst volumes in both reactors were minimized.

The range of chosen extents for the first reactor, 0.3 - 0.4 kmol s⁻¹, also proved to be robust, providing well performing reactors with small catalyst volumes (where all reactors had a combined catalyst volume less than half of that of the single stage reactor). Volume reached a minimum of 3.94 m³ when the extent was fixed at 0.34 kmol s⁻¹ with an inlet feed temperature of 737.1K.

5.3. Cold-shot Cooling

Table 4 - Conditions and results for the optimum cold-shot system

Extent Achieved

Temperature (K)

Catalyst volume (m³)

1st

2nd

1st

2nd

In

Out

In

Out

Vr1

Vr2

0. 2958

0. 2489

699

795. 769

717. 172

796. 407

1. 523

3. 254

($V_c 1$ & $V_c 2$ = 1st & 2nd Catalyst volume respectively)

Figure 11: Catalyst volume minimizing temperatures at specific alpha values

During simulation of the cold-shot cooling reactor design, it was deduced that the range of $\hat{\alpha}$ was restricted from 0. 01 to 0. 38, beyond which the bulk of the reaction would occur in one of the two reactors, making the other redundant. Optimally, $\hat{\alpha}$ should be somewhere between the limits of the range; for $\hat{\alpha} = 0. 19$ and feed temperature at 699K, a minimum overall volume of 4. 78 m³ was achieved. It is seen from the graph above that as $\hat{\alpha}$ deviates from 0. 19 and tends towards 0, the first reactor behaves more like a single PFR. The same happens to the second reactor as $\hat{\alpha}$ tends towards the $\hat{\alpha}$ upper limit.

Increasing the initial feed temperature causes \hat{I}_{\pm} to increase in order for optimization to occur, while a decrease would bring about the opposite effect. This is because a larger fraction would be required to cool the output from the first reactor to achieve optimization should the reactor operate at a higher temperature. The contrary is true; with a larger \hat{I}_{\pm} , the initial feed temperature cannot be too low as excessive cooling of the second fraction would occur.

6. Conclusion

It can be concluded that the investigation w