Dynamic Study of Feed-Effluent Heat Exchanger Addition on Double Bed Configuration Ammonia Reactor System within Varied Quenching Ratio

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Abstract. Ammonia is one of the most important industrial commodity due to its wide function. Ammonia synthesis reaction is an exothermic reaction. Therefore, Feed-Effluent Heat Exchanger (FEHE) is added to increase thermal efficiency. However, FEHE could lead the process to experience hysteresis phenomenon due to interaction between equipments as one steady state T feed could result several T outlet. Hysteresis phenomenon may result asset losses like explosion, leakage, and losing material integrity. Double bed reactor configuration allows us to use several operating parameters as variation to overcome hysteresis. In this review, quenching ratio was chosen to be that varied parameter. This study aims to determine how quenching ratio affects hysteresis zone by utilizing Aspen Hysys® V8.8 as simulation tool. Simulation showed that quenching ratio would narrow hysteresis zone yet increased extinction temperature that lower the conversion. Conversion profile showed that 0.2 quenching ratio got the highest conversion for system with bed volume ratio 2:1 while total volume was 30 m³. However, the feed temperature was fallen at hysteresis zone. Dynamic simulation showed that highest conversion feed temperature (10%ΔTf above extinct temperature) was still able to preserve stability with descending temperature approach. Hysteresis itself started to occur at 1.7%ΔTf above extinct temperature

1 Introduction

Ammonia is one of important industrial commodity due to its wide utilization as chemical product precursor such as urea, nitric acid, and etc. In ammonia production system, Feed-Effluent Heat Exchanger (FEHE) is commonly used that aims to exchange heat between reactor effluent and reactor feed as shown in Fig. 1.

Fig. 1. Ammonia reactor system configuration

Such heat integration system would reduce utility requirement and increase thermal efficiency. However, the integration system could possibly lead the process system to experience significant temperature oscillation as shown in Fig. 2. Oscillations occur as the result of two or more processes that are coupled together with each other [1,7]. In this case, reactors performance is closely related to how the FEHE performs. As the result, reactor possibly undergoes a phenomenon while same operating condition could produce several steady state outputs that lead the process to oscillate [1,6]. This condition could

cause several hazards for the equipment material and even operational staff [4,5]. Hazards that occurred could dangerously result disasters such as explosion or poisonous chemical leakage which causing economic losses.

Fig. 2. Hysteresis phenomenon on industrial scale ammonia reactor. [3]

Hysteresis area could be predicted by plotting one of steady state parameter such (T outlet) as result of T feed input as shown in Fig. 3.

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Fig. 3. Curve plot to determine hysteresis zone

The 'S' curve produced showed that within range of T_L and T_R (ΔT_f), each T_{feed} input will result several values of T_{outlet} . Therefore, there will be possibility for the process to experience oscillation while entering this region.

Some efforts to deal with this condition could be done by changing other supporting operation parameter for double bed system such as adding trim heat exchanger, bed volume distribution, or quenching ratio.

Therefore, this study would show parametric review and simulation regarding actions to overcome and reduce hysteresis phenomenon by choosing quenching ratio as varied operation parameter. As the quenching ratios were evaluated, conversion profile was also analyzed to map the best temperature at particular quenching ratio to produce optimum reactant conversion. As the matter of limiting the problem, this review focused on observing feed temperature, outlet reactor temperature, quenching ratio, reactant conversion, and starting hysteresis temperature.

2 Methods

Aspen Hysys® V8.8 were used to act as an assistive tools for simulating the dynamic behaviour resulted from altered parameter value. Simulation configuration is shown in Fig. 4.

Fig. 4. Simulation Configuration

Fluid package used in the simulation was Peng-Robinson. Ammonia reaction kinetics behaviour for calculation was based on following equation [2].

$$r = 23.618 \exp\left(-\frac{87,090}{RT}\right) \frac{P_{N_2} P_{H_2}^{1.5}}{P_{NH_3}} \quad (2)$$

$$- 3.39 \times 10^{13} \exp\left(-\frac{198,460}{RT}\right) \frac{P_{NH_3}}{P_{H_2}^{1.5}}$$

Plug Flow Reactor (PFR) with total volume 30 m^3 was used in the simulation. Quenching process was simulated by using splitter and mixer features of Aspen Hysys® V8.8. Quenching ratio was varied with assumed 1st bed volume at 20 m^3 and 2nd bed at 10 m^3 . FEHE simulation was conducted with steady-state-rating mode and sized rigorously by using interactive mode to obtain certain characteristic on heat transfer. FEHE specification sheet is shown in Table 1.

Hysteresis zone identification was conducted by using Adjust feature on Aspen Hysys® V8.8. This process was done by varying the 2nd reactor inlet temperature to adjust the feed temperature on each quenching ratio. This attempt eventually would result plot T_{Feed} vs T_{Outlet} correlation to identify hysteresis zone. Reactant conversion was then identified by using Case Study feature on Aspen Hysys® V8.8. This study was done by varying feed temperature on each quenching ratio or bed volume distribution and observing the mole flow of the ammonia in the outlet stream. At the end, Aspen Hysys® V8.8 Dynamic feature was conducted to observe the process dynamic behaviour at quenching ratio which resulted highest reactant conversion. Eventually, dynamic observation was used to determine starting temperature of oscillation as the percentage of ΔT_f . Dynamic simulation was also used to determine process stability while feed temperature was set at value that resulted highest conversion in chosen quenching ratio.

Table 1. FEHE Specification Sheet.

Specification	Value	Specification	Value
TEMA	AEL	Shell Diameter (mm)	818.85
Number of Shell per Pass	1	Number of Tube per Shell	872
Number of Shell in Series	1	Tube Pitch (mm)	23.81
Number of Shell in Parallel	2	Tube Layout Angle	Triangular (30°)
Tube Passes per Shell	1	Shell Fouling Factor ($^{\circ}\text{C m}^2/\text{kJ}$)	0.000028
Orientation	Horizontal	Baffle Type	Single
First tube pass flow direction	Counter	Baffle Orientation	Horizontal
Elevation	0	Baffle Cut (%Height)	20.00
Shell HT coeff. ($\text{kJ}/\text{m}^2\text{ }^{\circ}\text{C}$)	8908	Baffle Spacing (mm)	800.00
Tube HT coeff. ($\text{kJ}/\text{m}^2\text{ }^{\circ}\text{C}$)	12304	Tube OD (mm)	19.050
Overall U ($\text{kJ}/\text{m}^2\text{ }^{\circ}\text{C}$)	2604	Tube ID (mm)	10.668
Overall UA ($\text{kJ}/\text{m}^2\text{ }^{\circ}\text{C}$)	101900	Tube Thickness (mm)	4.191
Shell pressure drop (bar)	0.5855	Tube Length (m)	3.750
Tube pressure drop (bar)	0.1386	Tube Fouling Factor ($^{\circ}\text{C m}^2/\text{kJ}$)	0.000028
Heat transfer area per shell (m^2)	195.7	Thermal cond. (W/mK)	45
Tube volume per shell (m^3)	0.2923	Wall Heat Capacity Coeff. ($\text{kJ}/\text{kg }^{\circ}\text{C}$)	0.473
Shell volume per shell (m^3)	1.043	Wall Density (kg/m^3)	7801

3 Results

Unstable process as the result of FEHE utilization in double bed reactor is possible to create instability zone like the one in single bed configuration. Identified instability zone study resulted from varied quenching ratio and bed volume distribution of double bed reactor would be explained in the following section.

3.1 Hysteresis Zone Alteration Due to Varied Quenching Ratio

Fig. 5 shows that generally higher quenching ratio would lead to more narrow hysteresis but higher extinct temperature.

Fig. 5. Hysteresis zone alteration on varied quenching ratio

Higher extinct temperature could possibly lead the reaction to easily extinct and furthermore it would result lower reactant conversion. At bed volume distribution of 2:1, hysteresis zone experienced trend of rise from 0.1 to 0.2 and drop from 0.2 – 0.8. From here, there was an observed reversed trend at 0.2 quenching ratio. This possibly indicates that there was optimum point regarding the process parameter related to feed or outlet temperature. Closest relation to these parameters was conversion profile of the reaction. Reactant conversion was then evaluated from each quenching ratio at steady state simulation as shown in Fig. 6.

Fig. 6. Conversion profile on varied quenching ratio with 1st bed volume = 20 m³

Fig. 6 shows that generally lower quenching ratio will increase the conversion and it shows highest overall conversion profile at 0.2 quenching ratio. Optimum point of conversion profile at each quenching ratio was then plotted as shown at Fig. 7.

Fig. 7. Highest conversion plot at each quenching ratio

Fig. 7 shows that quenching ratio 0.2 resulted highest conversion which is 18.97% at bed volume distribution 2:1. This is the equilibrium conversion and obtained at $T_{\text{feed}} = 190^{\circ}\text{C}$. However, this temperature was located inside the hysteresis zone and was close to the 0.2 quenching ratio extinct temperature which was 184.69°C . Therefore, dynamic simulation then was conducted to determine the stability behaviour at 190°C as the operation is basically purposed to achieve conversion requirement as high as possible.

3.2 Dynamic Simulation

In this section, Aspen Hysys® V8.8 Dynamic Mode feature was utilized to identify stable/unstable behaviour in real time. From Fig. 5, we know that extinct temperature is 184.69°C at 0.2 quenching ratio. Hence, utilizing Dynamic Mode could possibly show minimum temperature to start hysteresis (as function of $\Delta T_f = 107.62^{\circ}\text{C}$) before the oscillation extinct the reaction. Dynamic Mode was started with igniting the reaction by set the T_{feed} to 300°C (refer to Fig. 8). T_{feed} was then lowered steppedly to 200°C and then 190°C . Starting from this point, feed temperature was lowered rampedly by 0.1°C to find the hysteresis minimum temperature as accurate as possible. Dynamic simulation showed that oscillation phenomenon started at 186.6°C . This means that at 0.2 quenching ratio and bed volume distribution 2:1, hysteresis mathematically will start approximately at:

$$T_{\text{feed hysteresis}} = T_{\text{extinction}} + 1.77\% (\Delta T_f) \quad (3)$$

Fig. 8. Minimum hysteresis temperature determination at 0.2 quenching ratio

Highest conversion while applying 0.2 quenching ratio and bed volume distribution 2:1 was obtained at 190°C . Mathematically this point was formulated as:

$$T_{\text{feed highest conversion}} = T_{\text{feed}} + 5\% (\Delta T_f) \quad (4)$$

Therefore, this feed temperature was tested in Dynamic Mode to measure whether the highest conversion could be achieved stably. Result is shown in Fig. 9. Referring to Fig 9, we are able to conclude that highest conversion of the reaction (at bed volume distribution 2:1) could be achieved stably.

Fig. 9. Stability identification at highest conversion feed temperature (190°C)

4 Conclusion

Quenching ratio alteration could affect how wide the hysteresis area is while plotting T_{outlet} vs T_{feed} . Higher quenching ratio showed narrowing hysteresis yet increase the extinct temperature that could lower the conversion. Highest conversion was obtained at 0.2 quenching ratio (bed volume distribution 2:1) with $T_{\text{feed}} = 190^{\circ}\text{C}$ which entering the hysteresis zone. However, this condition was chosen to be analyzed more in the Dynamic Mode to determine whether 190°C would already triggered the oscillation. Dynamic Mode showed that oscillation started at 186.6°C and further extinct the reaction. The highest conversion feed temperature was then tested in Dynamic Mode and resulted stable operation. Therefore, while using bed volume distribution 2:1 (total volume = 30 m^3), ammonia reaction highest conversion of 18.97% (quenching ratio = 0.2) is still able to be obtained at stable operation.

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