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Dynamic Simulation of an Ammonia Synthesis Reactor

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Abstract

In the ammonia synthesis process like most other processes the main processing unit and one that attracts most attention from a control point of view is the rector. In ammonia production plant there exists two reactors, the mathanation and the synthesis. The methanation reactor is of much less importance as little amount of reaction takes place in it, while the synthesis reactor is of outmost importance. In this paper initially a four-bed ammonia synthesis catalytic reactor is simulated in a dynamic environment. The simulation is then used to analyze the effect of sudden change on feed pressure and variation of feed distribution on different beds on process parameters such as temperature, pressure, flow rate and concentration through the process.

1. Introduction

Automatic and computer aided control of process plants is in practice for many years. This is due to the positive effects of computer control on a production line from a production engineer's point of view. It enables on line, fast and precise control of processes and it is much more valued when only fine controlling practice could be effective and possible. Automatic control of processes has been advancing in the technologies being used. The main tool on which computer aided process has been control is based is the dynamic model of the plant. A controlling practice can only be as effective in application as the model used for prediction is precise and exact. With a dynamic model the behavior of a process in time is predicted as a result of a wanted or an unwanted change on a process parameter. A dynamic process model may also be used for other purposes such as the design of start up and shut down procedures. With all this in mind the ammonia synthesis reactor has been simulated here and the simulation used for an in depth analysis of the process.

2. Kinetics of the Ammonia Synthesis Reaction

The ammonia synthesis reaction is an equilibrium reaction between hydrogen, nitrogen and ammonia, in the presence of magnetic iron oxide. The conversion is a function of pressure, temperature and the reactants ratio. Raising the reaction pressure increases the equilibrium conversion therefore increasing the heat of reaction produced inside the catalyst bed. This causes an increase in temperature resulting in a rise in spacial velocity. These results in a reduction in the reactor volume required compared to a reactor operating at lower pressure. The equilibrium reaction is defined by:

$$\frac{1}{2}N_2 + \frac{3}{2}H_2 \Leftrightarrow NH_3 \quad , \Delta H_{18^\circ C} = -11.0\,\text{Kcal} \quad , \Delta H_{629^\circ C} = -13.3\,\text{Kcal} \qquad (1)$$

The reaction is exothermic and the equilibrium rate constant is given by:

$$K_P = \frac{P_{NH_3}}{(P_{N2})^{\frac{1}{2}} \times (P_{H2})^{\frac{3}{2}}} \tag{2}$$

To describe the kinetics of this reaction in the gas phase, the equation type is selected to be equilibrium and reversible and the stocheometry of it is selected using standard equations. The equilibrium and rate constants as functions of temperature are given by:

$$LnK = 2.6899 - 5.5192\times10^{-5} + \frac{2001.6}{T} - 2.691LnT \quad , \quad k = 2.45\times10^{6}\exp\left(\frac{1.635\times10^{8}}{RT}\right) \tag{3}$$

When K is the equilibrium constant and k the rate constant.

3. Dynamic Simulation of the Ammonia Synthesis Reactor

As stated before a four bed catalytic fixed bed ammonia synthesis reactor has been simulated here in a process simulator environment. The choice of four fixed beds is to ensure the simulation is capable of providing on analysis tool for as complicated a reactor as exits in this process. The simulation is initially developed in a steady state environment. To do so the SRK thermodynamic package is used. The equations and the relating constants are defined as expressed before. The instrumentation and control devices and the relating parameters were then designed and installed on each of the streams and equipments. The simulation developed thus far is transferred into the dynamic environment. Fig.1 demonstrates the mechanism the four-bed reactor was simulated. As observed the main feed gas is divided into two stream one passing through the control valve (VLV-100) and the other bypassing it. The two join and enter the shell side of the preheater exchanger, entering the top of bed 1 after being heated up. The rest of the feed is sub-divided into four quenching streams. Each of the quench gas streams are pass through a separate control valve and fed on top of each of the four catalytic beds to control process operation. The final product exiting bed 4 is passed through the tube side of the feed preheater.

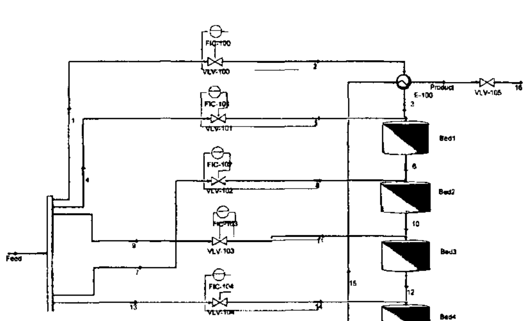


Fig1: the reactor mechanism simulated in the simulation environment.

4. Results and Discussions

Using the dynamic model developed some cases of interest are studied. They are reviewed below.

4.1. Case 1: The effect of sudden changes in feed pressure on process parameters

As observed in fig.2 a sudden increase in feed pressure of 5 bars initially results in an increase in feed flow rate passing through the 5 control valves. The feed flow rate increase through each of the valves is proportional to the initial flow passing though each under steadies state conditions. The controllers close the valves gradually to control the flow rate passing through resulting in the gradual reduction in the flow rates demonstrated in fig 2. A trend opposite to that described above is demonstrated in fig. 3 for a case of reducing the feed pressure by 5 bars. The changes on feed pressure affects reactor pressure and as the reaction takes place in the gas phase the ammonia produced is affected. The 5 bars increase causes an increase in the reactor pressure raising the reaction rate and therefore ammonia production rate as demonstrated on fig.4. The controlling effect of the values again reduces the molar ammonia flow rate. The opposite effect is observed in fig.5 for the case of sudden reduction in feed pressure of 5 bars. The smaller change shown on fig.5 as compared to fig.4 indicates that the reaction is less affected by pressure reductions compared to pressure increases. One of the process parameters of importance in controlling the reactor operation is the temperature of the streams leaving each of the four catalytic beds. In this simulation exit temperatures of the four beds are recorded and the plots are shown in fig.6 and fig.7. The temperature variations are very slight and therefore not of much significance on their effect on the overall operations. As expected the bed exit temperatures show an increase for the 5 bars pressure increase in the feed and a reduction for the reverse case. The larger temperature changes shown on bed 1 exit are dew to the fact that a larger portion of the reaction takes place in this bed compared to the other 3 beds.

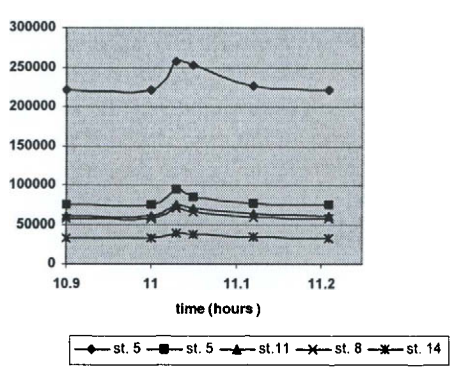


Fig.2: The effect of 5 bar pressure increase on mass flow rate of feed entering reactor beds.

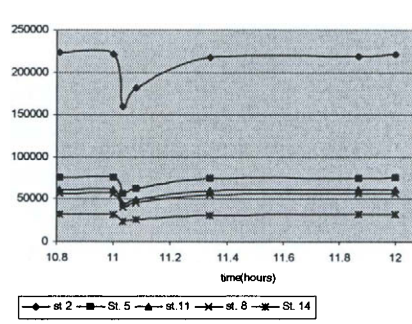
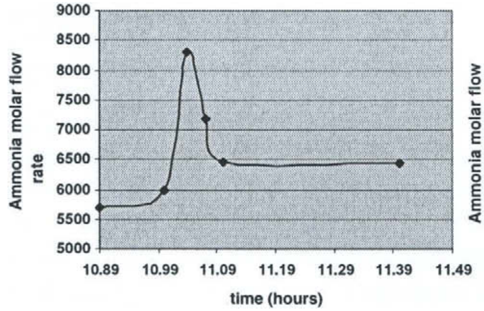


Fig3: The effect of 5 bar pressure decrease on mass flow rate of feed entering reactor beds.



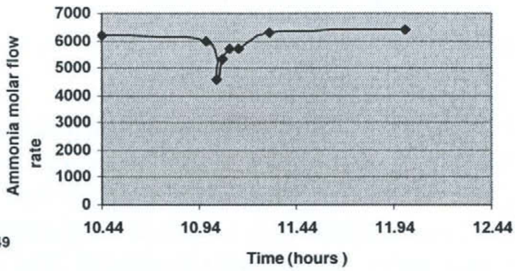


Fig4: The effect of 5 bars pressure increase on ammon a production.

Fig5: The effect of 5 bars pressure decrease on ammonia production.

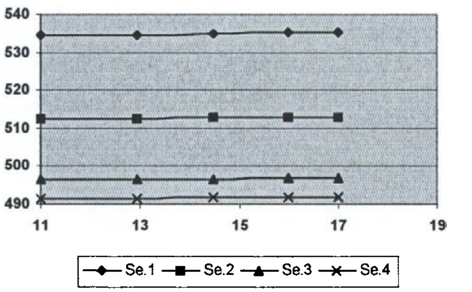


Fig6: The slight effect of 5 bars pressure increase on temperature of streams leaving the 4 beds.

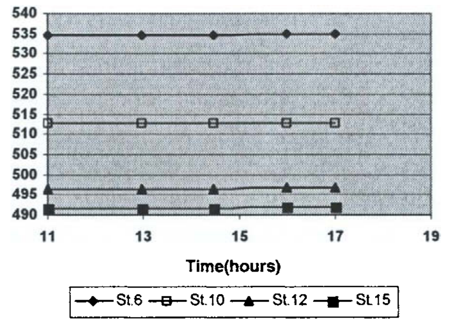


Fig7: The slight effect of 5 bars pressure decrease on temperature of streams leaving the 4 beds.

4.2. Case 2: The effect of feed distribution on the four beds on process parameters

As unlimited number of variations can be thought of when different percentages of feed distribution on each of the four catalyst beds are to be considered a change of feed to one bed may or may not be compensated for by variations of the flow rates on the other 3 beds. In the following two such cases studied by the simulation are described.

4.2.1. Case 2-1: Reduction of feed rate to bed 1 and a proportional compensative increase of feed rate on the other 3 beds

In this case study the feed rate being fed to bed 1 (the preheated flow) is reduced. Increasing the feed rate to the other three beds compensates the exact amount of reduction. The percentage distribution is given in table 1.

Table 1: feed distribution variation on the 4 catalytic beds for case 2-1.

Mass distribution of feed%	Feed entering bed 1after preheating	Feed entering bed1 without preheating	Feed entering bed 2 without preheating	Feed entering bed 3 without preheating	Feed entering bed 4 without preheating
Before change	49.52	16.82	12.7	13.68	7.18
After change	45.15	17.87	14.06	14.46	8.435

Fig. 8 demonstrates feed variations. The variations are carried out using the valve openings and due to this an initial overshot is observed in the increase of stream 2 and the decreases of the other four streams. Changes in the amount of value opening results in flow rate variations and therefore the pressure changes that affect flow rates so that initial settings are achieved. Fig.9 shows temperature variations caused as a result. This is partially due to lower overall temperature of main feed entering bed 1 as well as the larger quenching effect of the other non-preheated feed entering other beds. The overall reduction in reactor temperature as expected causes a better reaction propagation and therefore more ammonia produced as demonstrated in fig 10.

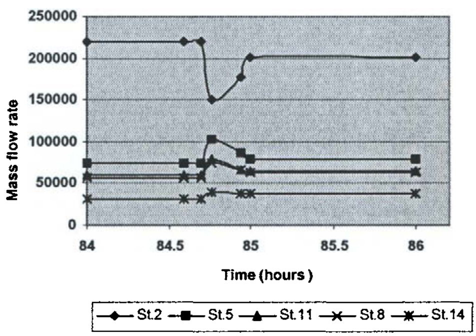


Fig8: Variation of feed entering the 4 beds in time according to case 2-1.

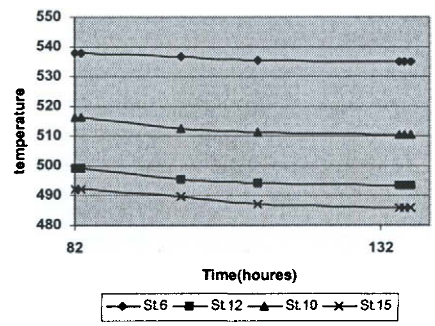


Fig9: The variation of temperature of stream leaving 4 beds according to case 2-1.

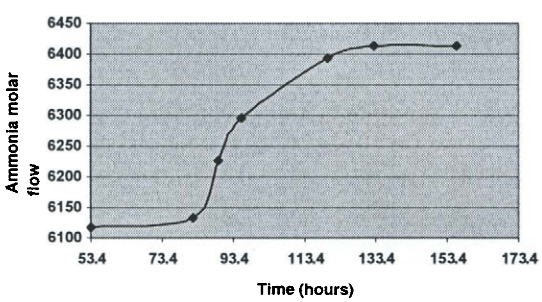


Fig10: Variation of ammonia produced by time as a result of changes in case 2-1.

4.2.2. Case 2-2: Increase in feed rate to bed 3 and a proportional and compensative decrease in the other 4 feed streams

The feed rate to bed 3 is drastically increased from 13.7% of the total feed to 21.85%. The increase is made up for by reduction on the other streams. The amounts of changes are given in table 2.Reduced feed rates to beds 1 and 2 results in an increase in temperature of stream leaving the two beds. This is shown in fig 11. The reverse is observed in the same plot for the temperature of bed 3 due to the increase of the feed rate to this bed. The temperature of stream leaving bed 4 is affected diversely by the reduction in the temperature of stream leaving bed 3 (causing a reduction in temperature of bed 4 product) as apposed to the reduction of the fresh feed entering bed 4 (causing an increase in temperature of bed 4 product). The sum effect is reduction in bed 4, product temperature. This is demonstrated in fig.11.As temperature variations are not significant production rates are not varied significantly. Only slight increase in overall ammonia production is observed as shown in fig.12.

Table2: feed distribution variation on the 4 catalytic beds for case 2-2.

Mass distribution of feed%	Feed entering bed 1after preheating	Feed entering bed.1 without preheating	Feed entering bed 2 without preheating	Feed entering bed 3 without preheating	Feed entering bed 4 without preheating
Before change	49.53	16.89	12.7	13.7	7.16
After change	45.2	15.67	11.24	21.85	6.02

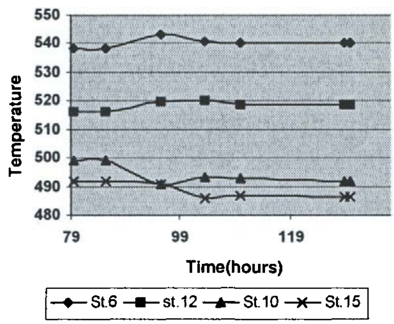


Fig11: The variation of temperature of stream leaving 4 beds according to case 2-2.

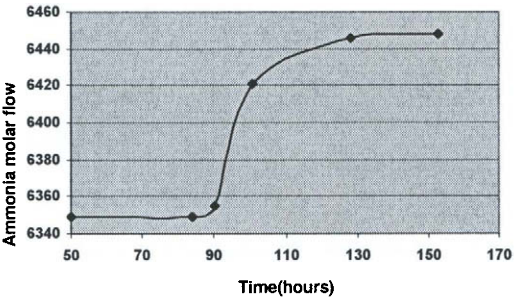


Fig12: Variation of ammonia produced by time as a result of changes in case 2-2.

5. References

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