

MATHEMATICAL SIMULATION OF ADJACENT-COUPLING AMMONIA ABSORPTIVE REACTOR.

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ABSTRACT

The development of an efficient process for ammonia synthesis is a goal that has been long sought after; therefore, the application of an absorptive reactor for ammonia synthesis is important since it allows the reaction to occur under milder conditions. In the adjacent-coupling absorptive reactor, absorbent particles are positioned downstream the fixed ammonia synthesis catalyst bed. This kind of absorptive reactor leads to the enhanced conversion of ammonia synthesis under milder conditions, compared to the equivalent reactor used without absorbent. Here, we present the transient backflow cell model (BCM) to explain and analyse the phenomenon of absorption-enhanced reaction. The transient BCM, based on the first principle of mass balances, is developed to simulate that the backflow existing through the absorptive reactor. As a reference, the transient cell model (CM) is also implemented to simulate the absorptive reactor when assuming no existing backflow existing. These two models demonstrated that backflow through the absorptive reactor promotes the ammonia reaction conversion via two mechanisms: longer residence time for reaction and faster reaction rate due to the absorption of ammonia absorbed.

1. INTRODUCTION

Ammonia synthesis through the Haber-Bosch process is widely recognised as one of the most significant industrial applications (Bruce and Faunce 2015). Gas reactants hydrogen and nitrogen are converted to ammonia, operating in a catalytic packed bed reactor under high pressure (150-250 bar) and high temperature (400-500°C) (Appl 1999). Due to the problems of low single-pass conversion and energy-intensive operating conditions, the development of an ammonia synthesis reactor to enhance single-pass product yield and to adapt technology to and a less energy-intensive operation has attracted much attention.

A small number of research studies have investigated using the absorptive reactor to improve ammonia synthesis (Huberty et al. 2012; Wagner et al. 2017; Smith et al. 2019). The ammonia synthesis was enhanced by magnesium chloride absorption (Huberty et al. 2012), as the composite absorbents based on chlorides of alkaline-earth metals have a high ammonia absorption capacity (Zhu et al. 2009). Column absorption for reproducible cyclic separation in small scale ammonia synthesis was introduced in (Wagner et al. 2017). C. Smith et al. even ran the reaction and absorption at one temperature in the same piece of process equipment (Smith et al. 2019). However, no research focuses on the case when the catalyst bed and absorbent beds are sequentially packed in one column. In this paper, we focused on this adjacent-coupling configuration of the absorptive reactor for ammonia synthesis. As an increase in conversion was measured experimentally, it can be concluded that the flow regime is not an ideal plug flow, but backflow exists through the reactor. In this paper, the backflow is proposed to explain the absorption-enhanced conversion of ammonia synthesis. The reason for the improvement of the conversion will be identified in this paper. The transient backflow cell model (BCM) for the absorptive reactor was created to specify or verify the extent of absorption effect and determine the most efficient absorbent amount. The backflow cell model has actually been adopted in many types of research before (McSwain and Durbin 1966; Sinkule et al. 1976). The backflow cell model is of convenient because the mathematical treatment is simple, as shown by a numerical investigation for multiple stages. The transient backflow cell model (BCM), based on the first principle of mass balances, was developed and implemented in MATLAB®. Meanwhile, the transient cell model (CM) was implemented as a reference to simulate the absorptive reactor when assuming no backflow and, therefore, no absorption effect. The sensitivity on the number of cells, as one parameter used in the model, is also considered.

2. EXPERIMENTAL SECTION

The synthesis of Cs-Ru/MgO followed the incipient wetness impregnation procedure. The effect of the absorbent on ammonia production was tested in a fixed-bed continuous-flow reactor using Cs-Ru/MgO catalyst. A glass reactor tube (cross-sectional area $5.024 \times 10^{-5} \text{ m}^2$) was packed with 0.1 g Cs-Ru/MgO catalyst and 1 g absorbent (MgCl_2) with quartz wool in between. A 3:1

mixture of H₂ and N₂ was passed through the reactor at a pressure of 10 bar and a weight hourly space velocity of 36000 mL g⁻¹ h⁻¹. The reactor was equipped with three independent furnaces that allowed different sections to be heated to different temperatures. Each furnace was controlled by an independent thermocouple. The middle thermocouple was directly inserted into the catalyst bed and was set to synthesis temperature. During the reaction step, the catalyst was at 400 °C and the absorbent at 150 °C. Finally, any ammonia absorbed on the absorbent was desorbed by heating the absorbent to 400°C under flowing nitrogen at ambient pressure. The reaction rate of the catalyst was 7884 μmolg⁻¹h⁻¹ with the absorbent loaded behind the catalyst and 5082 μmolg⁻¹h⁻¹ without the absorbent.

3. MATHEMATICAL MODEL

The backflow process leads to two possible mechanisms that affect the single-pass conversion of the reaction: increased residence time and ammonia removal due to the absorption effect. In this section, we identify and compare the extent of each mechanism via two models: the transient BCM and the transient CM for the absorptive reactor (catalyst bed adjacent to an absorbent bed) and the conventional reactor (catalyst bed only). Figure 1 represents a schematic of the transient BCM in an absorptive ammonia synthesis reactor.

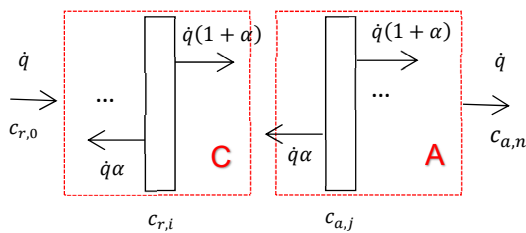


Figure 1: Schematic Diagram of the BCM in the Ammonia Synthesis Absorptive Reactor ('C' refers to the catalyst bed while 'A' refers to the absorbent bed).

The BCM hypothesises a stable unchanging backflow, expressed by $\dot{q}\alpha$ between each cell, to characterise the backflow mechanism in the reactor. There are m cells in the catalyst bed and n cells in the absorbent bed. In this case, the backflow ratio α represents the backflow amount. An α of zero is the plug flow limit; while when α equals infinity, the equations model approaches the stirred tank limit. The assumptions that govern the development of transient BCM are as follows:

- Due to symmetry in the radial direction of the packed bed, the governing equations are independent of this direction. Thus, a one-dimensional model is considered.
- Constant actual (interstitial) velocity is assumed.
- Isothermal condition is assumed in the catalyst bed.
- Each cell is assumed to be perfectly mixed.

- The volumetric flow of gas is assumed to be constant throughout the axial position of the bed.
- Instantaneous equilibrium of the solute in the bulk fluid with the absorbate.
- Catalyst/absorbent packing has uniform voidage and particle size.

According to these assumptions, the differential equations of the transient BCM were developed along the axial direction based on the principle of mass balance. The mathematical relationship for these cells can be written as follows. For the first cell of the catalyst bed:

$$V_{r,f} \cdot \frac{dc_{r,1}}{dt} = \dot{q}c_{r,0} + \dot{q}\alpha c_{r,2} - \dot{q}(1 + \alpha)c_{r,1} + V_{r,c} \cdot R_r \quad (1)$$

Similarly, the modelling equations for the intermediate cells of the catalyst bed ($i = 2, 3, \dots, m-1$) can also be written.

$$V_{r,f} \cdot \frac{dc_{r,i}}{dt} = \dot{q}(1 + \alpha)c_{r,i-1} + \dot{q}\alpha c_{r,i+1} - \dot{q}(1 + 2\alpha)c_{r,i} + V_{r,c} \cdot R_r \quad (2)$$

For the last cell of the catalyst bed:

$$V_{r,f} \cdot \frac{dc_{r,m}}{dt} = \dot{q}(1 + \alpha)c_{r,m-1} + \dot{q}\alpha c_{r,m+1} - \dot{q}(1 + 2\alpha)c_{r,m} + V_{r,c} \cdot R_r \quad (3)$$

For the first cell of the absorbent bed:

$$V_{a,f} \cdot \frac{dc_{a,1}}{dt} = \dot{q}(1 + \alpha)c_{a,0} + \dot{q}\alpha c_{a,2} - \dot{q}(1 + 2\alpha)c_{a,1} + V_{a,c} \cdot R_a \quad (4)$$

For the intermediate cells of the absorbent bed, $j = 2, 3, \dots, n-1$:

$$V_{a,f} \cdot \frac{dc_{a,j}}{dt} = \dot{q}(1 + \alpha)c_{a,j-1} + \dot{q}\alpha c_{a,j+1} - \dot{q}(1 + 2\alpha)c_{a,j} + V_{a,c} \cdot R_a \quad (5)$$

For the last cell of the absorbent bed:

$$V_{a,f} \cdot \frac{dc_{a,n}}{dt} = \dot{q}(1 + \alpha)c_{a,n-1} - \dot{q}(1 + \alpha)c_{a,n} + V_{a,c} \cdot R_a \quad (6)$$

where \dot{q} is the inlet gas flowrate (in m³/s) and $\dot{q}\alpha$ is the backflow. The forward flow increases to $\dot{q}(1 + \alpha)$. The mass balances for hydrogen, nitrogen, and ammonia are respectively calculated by Equations (1) through (6), with different reaction rates and absorption rates.

Dyson and Simon modified the Temkin expression to calculate the intrinsic rate of reaction in kmol/m^3 (Dyson & Simon 1968), given in Equation (7):

$$R_{r,NH_3} = 2k_2 \left[K_a^2 a_{N_2} \left(\frac{a_{H_2}^2}{a_{NH_3}^3} \right)^\beta - \left(\frac{a_{NH_3}^2}{a_{H_2}^3} \right)^{1-\beta} \right] \quad (7)$$

The parameter β is a constant, taking values between 0.5 and 0.75, and the expression of the activity of the components, a_k , is shown in Equation (8):

$$a_k = \frac{f_k}{P^0} = \frac{\phi_k y_k P}{P^0} \quad (8)$$

P^0 is the reference pressure and is assumed to be atmospheric (1 bar). Gillespie and Beattie calculated the equilibrium constant, K_a , and proposed the correlation in Equation (9) (Gillespie and Beattie 1930):

$$\log_{10} K_a = -2.691122 \log_{10}(T) - 5.519265 \times 10^{-5} T + 1.848863 \times 10^{-7} T^2 + \frac{2001.6}{T} + 2.689 \quad (9)$$

In turn, k_2 is estimated by the Arrhenius equation (Gillespie & Beattie 1930):

$$k_2 = 8.849 \times 10^{14} e^{\left(\frac{-40765}{1.9877} \right)} \quad (10)$$

The absorbents only absorb ammonia. Therefore, the absorption rate for hydrogen and nitrogen is zero.

In this mathematical model, the absorbent bed is first assumed to be in the non-saturated condition. Then, the saturation condition of the absorbent is additionally considered to determine the influence of the absorbent amount. While a detailed mechanism for absorption is not known, kinetic experiments conducted previously (Smith et al. 2018) allow the fitting of an analytical equation:

$$r_{abs} = k_{a1} e^{k_{a2}(P_{NH_3} - P_{NH_3}^+)} \text{ when } (P_{NH_3} - P_{NH_3}^+) < 1 \text{ bar} \quad (11)$$

$$r_{abs} = k_{a3} (P_{NH_3} - P_{NH_3}^+)^2 \text{ when } (P_{NH_3} - P_{NH_3}^+) > 1 \text{ bar}$$

where r_{abs} is the rate in micromoles per second per gram of absorbent, k_{a1-a3} are experimentally determined constants (Smith et al. 2019), P_{NH_3} is the pressure of ammonia in kPa, and $P_{NH_3}^+$ is the equilibrium pressure of ammonia at a given temperature in kPa, as illustrated in (Smith et al. 2019). Based on these analytical equations, the temperature profile of the absorbent bed could be

ignored as the parameters and equations were assumed to be independent of temperature-irrelevant.

The governing equation for the conventional reactor in BCM is Equation (12). To some extent, the existing of backflow can be assumed as that the flow goes through the catalyst bed with longer residence time. Therefore, the cell number of the catalyst bed is m' , which is higher than m .

$$V_{r,f} \cdot \frac{dc_{r,i'}}{dt} = \dot{q}c_{r,i'-1} - \dot{q}c_{r,i'} + V_{r,c} \cdot R_r \quad (12)$$

In the CM of the absorptive and the conventional reactors, the reactants flow in one direction. The modelling equations for the cells of the catalyst bed were consistent with Equations (1) to (6) but ignored the backflow.

4. SIMULATION AND DISCUSSION

The governing equations of the transient BCM and transient CM are ordinary differential equations which were solved using the ode15s solver from MATLAB®. The numerical results and discussion are presented in this section. Nitrogen is taken as the reference to calculate the reaction conversion.

4.1 The Conventional Reactor

Figure 2 depicts the concentration of these three components in the catalyst bed at different times (arrow points in the direction of an increasing number of cells). The steady-state concentration of hydrogen and nitrogen for the downstream position is lower than upstream positions as the reaction progresses.

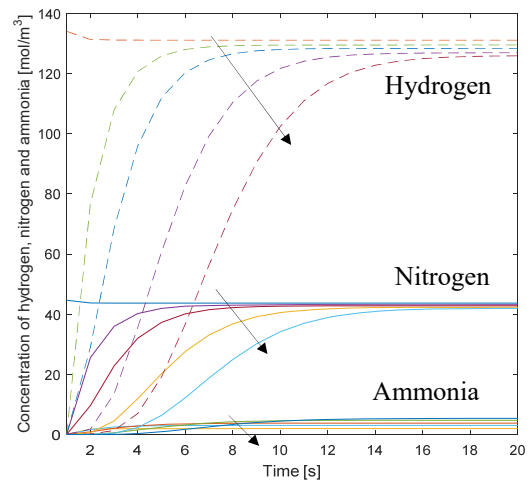


Figure 2: Concentration of hydrogen, nitrogen, and ammonia in the conventional reactor.

As illustrated in Figure 3, the concentration of ammonia increases from the first cell to the end as a result of the superposition of the produced ammonia (arrow points in the direction of an increasing number of cells). The

conversion in the catalyst bed is 6.25% according to the simulation results, which depend on the parameters used in the model, such as the length of the catalyst bed, temperature, and pressure.

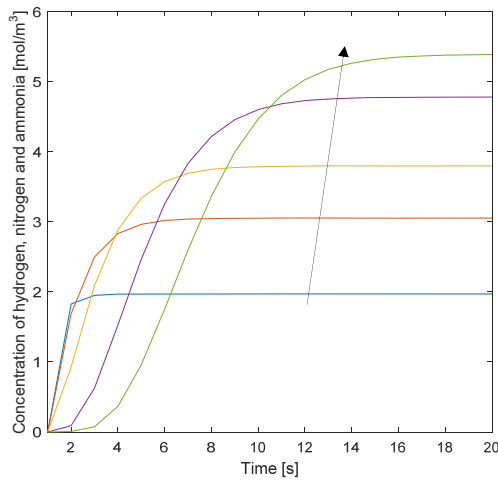


Figure 3: Concentration of ammonia in the conventional reactor.

Therefore, the reaction equilibrium has not been reached, as the thermodynamic equilibrium conversion of ammonia synthesis from $H_2: N_2 = 3:1$ at $T = 400\text{ °C}$ and $P = 10\text{ bar}$ is 7.45% (Ogura et al. 2018). Then, the effect of the catalyst bed length on the reaction conversion was considered here. As demonstrated in Figure 4, the conversion of the ammonia synthesis rises sharply at first with the increasing length of the catalyst bed, then reaches a stable value: the equilibrium point of this reversible reaction. This balance cannot be broken unless the reaction conditions change. In Figure 4, the ammonia synthesis reaches the equilibrium when the catalyst bed is longer than 0.04 m. The synthesis conversion is independent of the residence time if the equilibrium has been reached.

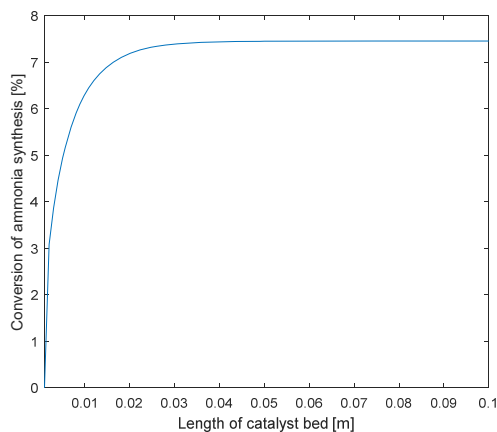


Figure 4: Variation of the conversion of ammonia synthesis with the length of the catalyst bed.

Figure 5 presents the conversion of ammonia synthesis under various backflow extents (0% to 100%) when the

length of the catalyst bed is 0.01 m. An increase in ammonia production conversion from 6.25% to 7.25% can be observed. In the transient BCM of the conventional reactor, the extent of backflow was assumed to be related to the number of cells in the catalyst bed, which replace the increase in residence time. When the extent of backflow is 100% the catalyst bed is assumed to be extended by about 10 cells, which means the flow has a longer residence time for reaction.

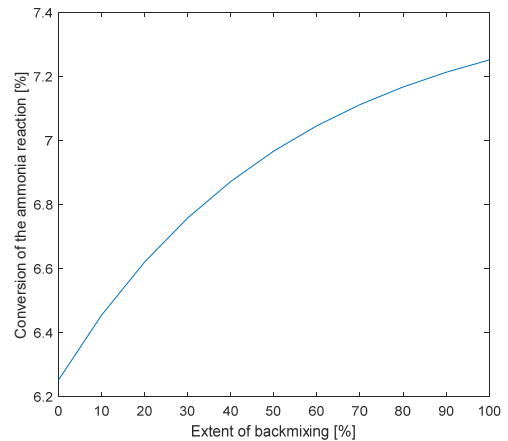


Figure 5: Effect of backflow on the ammonia synthesis conversion.

The number of cells is an important parameter in the BCM and CM. Therefore, it is necessary to analyse the sensitivity of the number of cells at a fixed-length catalyst bed, which is displayed in Figure 6 (arrow points in the direction of an increasing bed length). The cell number sensitivity study is a significant aspect to avoid inaccurate results due to an ill-conditioned cell number. In Figure 6, the cell number should be larger than 8 when the length of the catalyst bed is longer than the equilibrium length, and then the results stop changing with cell number. When the length of the catalyst bed is shorter than 0.04 m, increasing the number of cells will slightly increase the reaction conversion. Therefore, in this case, a cell number of 12 is taken to minimise the deviation of cell number dependence.

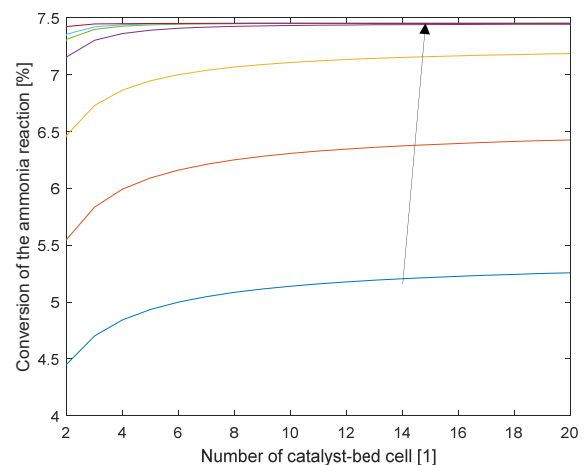


Figure 6: Sensitivity on the number of cells in the catalyst bed.

4.2 The Absorptive Reactor

Based on the results in Section 4.1 for the simulation of the absorptive reactor, the length of the catalyst bed was fixed to 0.1 m to ensure that the reaction equilibrium was reached and the cell number was set to be 8 to decrease computation time. The single-pass conversion of the absorptive reactor is 7.45%, calculated by the transient CM, which is the same as the conversion of the conventional reactor (0.1 m length). Therefore, the absorption does not affect the ammonia synthesis conversion when using the transient CM, which is not consistent with the experimental results.

Based on the experimental results, an absorption bed following the catalyst bed has an impact on the single-pass reaction conversion. Therefore, the transient CM does not apply to the absorptive reactor and the simulation can be switched to the transient BCM with a fixed 50% backflow ratio. The solid lines in Figures 7 and 8 display the concentration profiles of nitrogen and ammonia. Unlike the transient CM results (dashed lines), the ammonia concentration decreases at the end of the catalyst bed, when the flow has yet to reach to absorbent bed. The nitrogen concentration has a second drop at the junction of the catalyst bed and absorbent bed, shown in the red square of Figure 7.

The comparison of the transient BCM and CM simulations is illustrated in Figures 7 to 8 for a 50% backflow ratio. The arrows point in the direction of increasing time. As illustrated in Figures 7 and 8, the dashed curves and solid curves are noticeably different, which means that simulated results were influenced greatly by the backflow setting. Under the same cell number and same time conditions, a lower nitrogen concentration with higher ammonia concentration is revealed for the absorptive reactor with the BCM simulation in comparison with that in the CM simulation. This implies that the single-pass synthesis conversion in the BCM simulation is higher than the one predicted by the CM simulation. Undoubtedly, the transient BCM matched experimental results better than transient CM.

Based on the BCM simulation, the absorption capacity of the absorptive reactor, which promotes the reaction conversion, can be further analysed. In this BCM simulation, the equilibrium of the reaction in the catalyst bed has been reached as its length is set at 0.1 m with 8 cells. Therefore, the single-pass conversion of ammonia synthesis does not change when there is the only backflow without absorption or increased residence time, based on the results of Section 4.1. Therefore, the reason for improved conversion is due to the absorption capacity of the absorptive reactor, which speeds up the reaction rate and drives the reaction equilibrium as the partial pressure of ammonia decreases. Then, the backflow ratio,

length and cell number of absorbent bed, as well as the saturation degree of absorbent bed, will be discussed.

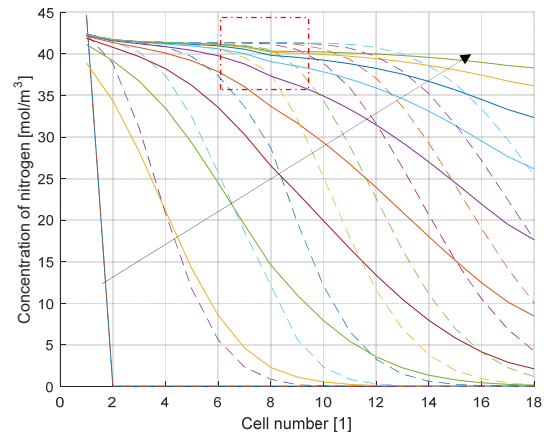


Figure 7: Concentration of nitrogen with respect to the position in the absorptive reactor.

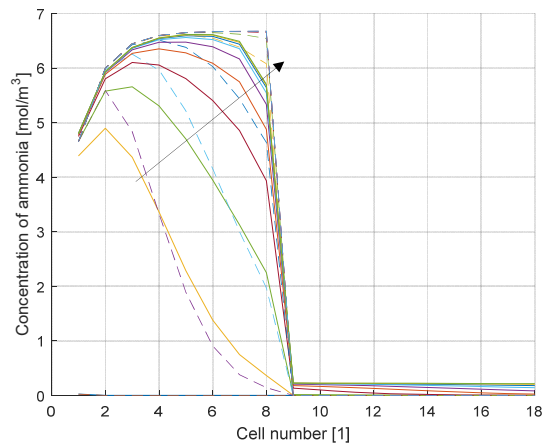


Figure 8: Concentration of ammonia with respect to the position in the absorptive reactor.

Figure 9 reveals a relationship between the synthesis conversion of the absorptive reactor and the backflow ratio. The reaction conversion has a linear growth as the backflow ratio increases when the absorbent bed has not been saturated. The reaction conversion increases from 7.45% (the equilibrium conversion) to 11.2% in Figure 9. Therefore, the absorption in the absorptive reactor can drive the synthesis equilibrium in the right direction when the thermodynamic equilibrium of the reaction has already been reached.

Then, the length and cell number of the absorbent bed were considered for their impact on the conversion improvement. Based on the simulation results, it is illustrated that increasing infinitely the length or the cell number of the absorbent bed does not affect the synthesis conversion when the absorbent bed was assumed to be unsaturated.

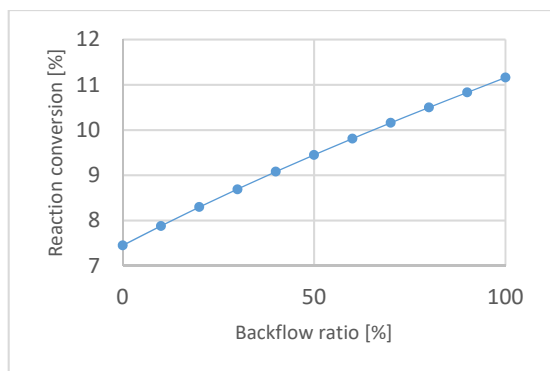


Figure 9: Relationship between reaction conversion and backflow ratio in the absorptive reactor.

However, in reality, the absorbent bed is gradually saturated as the synthesis take place, and the effect of absorption on the synthesis conversion begins to wane as the absorbent pellets stop absorbing ammonia. For example, Figure 10 displays a relationship between the absorptive reactor conversion and the saturated cells in the absorbent bed. In this case, the backflow ratio is set at 50% with a fixed-absorbent-bed length of 0.1 m. A saturated cell number equal to six means that the first six cells of the absorbent bed have been saturated and the absorption occurs at the third cell. Figure 10 reveals that the saturation state of only the first six cells in the absorbent bed can affect the synthesis conversion. Once the first six cells are saturated, the conversion no longer increases, and there is no difference between an absorptive reactor and a conventional reactor.

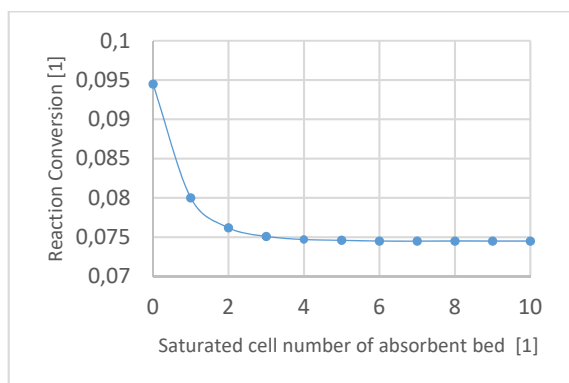


Figure 10: Reaction conversion of ammonia synthesis with a gradually saturated absorbent bed.

When the ammonia synthesis in the catalyst bed has not reached the thermodynamic equilibrium, the results indicate that, under the kinetically controlled regime, both the longer residence time and the absorption of ammonia can yield higher ammonia conversion to approach the thermodynamic value as shown in our model. If the packing after the catalyst bed contains solid pellets but no absorbent, the reaction conversion can be improved only by the residence time. However, once the equilibrium is reached, the increase of the reaction conversion is due to the absorption. The backflow ratio

can be regarded as the scale of the fluid disorder in the absorptive reactor, which will directly relate the impact extent of absorption on synthesis. If the backflow ratio is zero, the decrease in ammonia concentration or partial pressure due to absorption will not affect the synthesis reaction. Furthermore, when the backflow ratio is one hundred, the reactants with the reduced partial pressure of ammonia (ammonia was absorbed) will flow to upstream cells, speeding up the reaction and driving the equilibrium.

It can be summarized that the reaction conversion is entirely independent of the cell number of the absorbent bed. Once the absorbent bed length is long enough, e.g. at least 0.1 m, the reaction conversion will not increase even if the absorbent bed is longer. Moreover, if the first several cells (about 0.06 m) of the absorbent bed are saturated, the absorption will not affect the synthesis conversion any more.

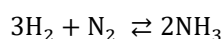
The reaction conversions for experimental results were 1.09% and 0.71%. These were much lower than the simulation conversion of a stoichiometric feed, which was due to the activity of the catalyst being calculated based on an iron catalyst (Dyson and Simon 1968) in the simulation, not on the Ru catalyst that was used in the experiment as the lack of rate expression for Ru catalyst. Furthermore, the data at mild conditions were not a good comparison for the reaction rates under ideal simulation conditions. However, as the backflow effects on the single-pass conversion in the simulation have the same increasing trend as in reality, this model of the ammonia absorptive reactor can, to some extent, explain the experimental results.

There are potential limitations to this simulation. In reality, both ammonia synthesis and absorption are highly exothermic. However, in this simulation, we assumed that the temperature of the catalyst bed was constant at 400 °C, while it declined linearly at the beginning of the absorbent bed from 400 °C to 150 °C. Also, the ammonia synthesis reaction is not equimolar (with 4 mol of reactants being converted to 2 mol of products), and absorption will only remove ammonia from the gas phase. In this simulation, the single-pass conversion of the reaction is quite low at about 5 – 7 %. Therefore, the volume change during the reaction and absorption processes was low enough to be ignored in this paper. Nevertheless, these are future simulation we would like to perform.

5. CONCLUSION

In this paper, a transient BCM was performed to simulate an absorptive reactor for ammonia synthesis. Meanwhile, the transient CM was taken as a reference to identify what role the absorbent plays in the enhancement of synthesis conversion. Modelling results indicate that the absorbent packed adjacently after the catalyst significantly affects the single-pass synthesis conversion through increased

residence time and faster reaction rate, driving equilibrium to the right. The backflow increases the residence time, while the faster reaction rate and equilibrium-shift are due to the reduced ammonia partial pressure (absorbed in the absorbent). The bench-scale absorptive ammonia synthesis reactor was operated to obtain experimental data to underline this point. Furthermore, the absorption has more impact on the conversion improvement than the increased residence time, as the proportional increase in Figure 9 is more significant than that in Figure 5. These two models could demonstrate that backflow in the absorptive reactor promotes the ammonia reaction conversion via two mechanisms: longer residence time for reaction and a faster reaction rate, driving the equilibrium of the reaction to the right (reversible reaction shown as below).



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