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Modeling and Simulation of Ammonia Synthesis in Fluidized Bed Reactor

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ABSTRACT

In this pater a fluidized bed reactor for ammonia convertor has been modeled. The achieved model is two phase model for the fluidized bed rectors based on some assumptions which simulate the reality, and the model equations have been solved using MATLAB. The reactor performance has been tested for some operating conditions to determine the effect of these operating parameters on the reactor performance. The results have been compared with the available industrial data; the comparison shows that there is 53% increase in nitrogen conversion when considering fluidized bed reactor.

Keywords: Ammonia, Modeling, Simulation, Fluidized bed.

1. INTRODUCTION

Ammonia is mainly used in the production of liquid fertilizer solutions which consist of ammonia, ammonium nitrate, and urea and aqua ammonia. It is also used in the manufacture of nitric acid, neutralizing the acid, several areas of water and wastewater treatment, stack emission control systems, industrial refrigeration systems, rubber industry, pulp and paper industry, food and beverage industry, leather industry, and other uses [1].

Modeling and simulation can play an important role to give an insight of the industrial units and hence simulation of Ammonia unit is very important to help investigating the different operation modes of this unit and optimize that.

2. Modeling of Fluidized Bed Reactors

The fluidized-bed reactor has the ability to process large volumes of fluid. For the catalytic cracking of petroleum naphtha to form gasoline blends.

Their main characteristics are:

1. Negligible diffusion resistances within the catalyst particles.
2. High heat and mass transfer rates between gas and particles.
3. Low pressure drop.
4. Large capacity.
5. Isothermality due to mixing by bubbles.

Fluidization occurs when small solid particles are suspended in an upward flowing stream of fluid, as shown in Figure [2].

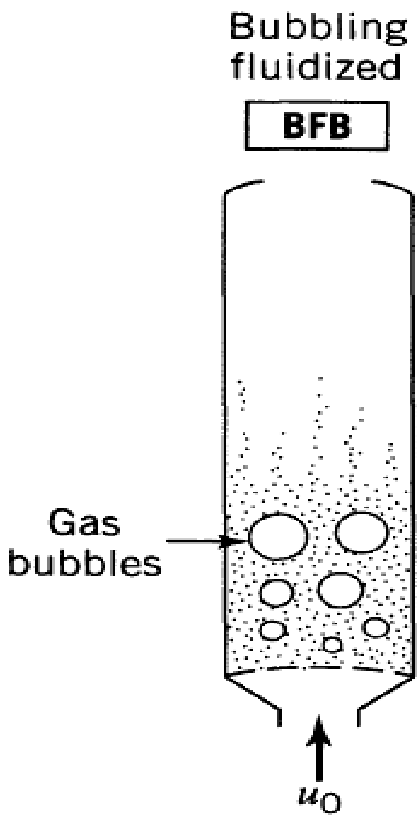

Fig 1: Fine powder inside a tube starting to fluidize due to gas flow rate [3]

3. Descriptive Behavior of a Fluidized Bed – The Two Phase Model

At gas flow rates above the point of minimum fluidization, a fluidized bed appears much like a vigorously boiling liquid; bubbles of gas rise rapidly and burst on the surface, and the emulsion phase is thoroughly agitated [4]. The bubbles form very near the bottom of the bed, very close to the distributor plate and as a result the design of the distributor plate has a significant effect on fluidized-bed characteristics.

Literally hundreds of investigators have contributed to what is now regarded as a fairly practical description of the behavior of a fluidized bed; chief among these is the work of Davidson and Harrison. Early investigators saw that the fluidized bed had to be treated as a two-phase system – an emulsion phase and a bubble phase. The bubbles contain very small amounts of solids. They are not spherical; rather they have an approximately hemispherical top and a pushed-in bottom. The two-phase theory of fluidization, states that “Almost all the gas in excess of that necessary for minimum fluidization will appear as gas bubbles” [10].

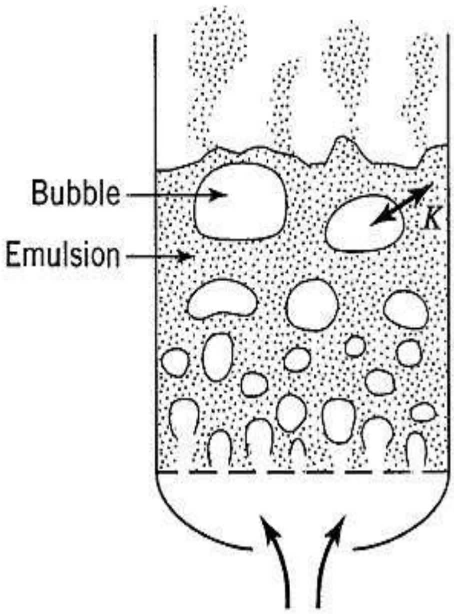

Fig 2: Phases of fluidized bed

4. Model Assumptions

The mathematical model is developed based on the two phase reactor model. The following assumptions are used to simplify the model equations [5]:

- The system is isothermal and steady state conditions.
- The lower dense bed assumed to compose of bubble and emulsion phases.
- The gas in the bubble phase is assumed in plug flow.
- The dense phase is assumed to be perfectly mixed.
- Reaction occurs mostly in the dense phase.
- Negligible mass and heat transfer resistances between the catalyst particles and the emulsion phase gas.
- Negligible heat of adsorption.

5. General Model Formulation

Based on the two-phase model, a fluidized catalytic bed reactor can be divided into two regions [6]; the dense phase (the emulsion phase), and the bubble phase with associated mass and heat transfer between the two regions and phases.

Consider the following simple reaction:

$$A \rightarrow R$$

Since the dense phase is assumed to be perfectly mixed, the concentration of the reactant (A) C_{Ad} will be constant for all height, while its concentration in the bubble phase which is assumed to be in plug flow C_{Ab} will be a function of the height h.

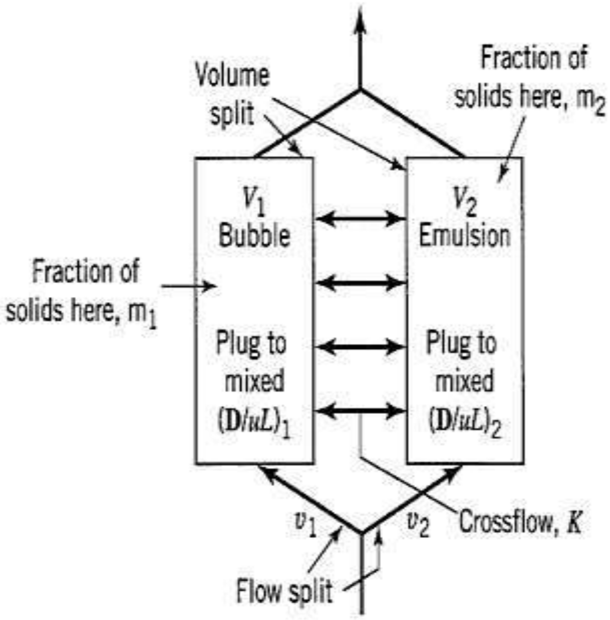

Fig 3: The two phases of fluidized bed

Where:

C_{Ad} is the concentration of component A in the dense phase

C_{Ab} is the concentration of component A in the bubble phase

5.1 Steady-state modeling of the bubble phase

Assuming that there is a negligible rate of reaction for an element in plug flow mode in the bubble phase, the molar balance can be expressed as [7]

$$\frac{dN_{jd}}{dz} = (K_{bd})_j \left(\frac{N_{jd}}{Q_d} - \frac{N_{jb}}{Q_b}\right) A_b \qquad (1)$$

With the initial conditions $N_{jb} = N_{jbF}$ at $z = 0$. Equation (1) can be solved analytically to give:

$$\frac{N_{jb}}{Q_b} - \frac{N_{jd}}{Q_d} = \left(\frac{N_{jbF}}{Q_b} - \frac{N_{jd}}{Q_d}\right) e^{-a_j z} \qquad (2)$$

$$a_j = \frac{(K_{bd})_j}{U_b} \qquad (3)$$

An energy balance for the bubble phase is given by:

$$\rho_g C_{pg} U_b \frac{dT_b}{dz} = (H_{bd})_b (T_d - T_b) \qquad (4)$$

With the initial conditions $T_b = T_F$ at $z = 0$. the equation (4) can be solved analytically to give:

$$T_b = T_d - (T_d - T_F)e^{-bz} \qquad (5)$$

$$b = \frac{H_{bd}}{\rho_g C_{pg} U_b} \qquad (6)$$

5.2 Steady-state modeling of the dense phase

The molar balance on the dense phase for component A gives:

$$N_{jd} = N_{jdF} + \int_0^H (K_{bd})_j \left(\frac{N_{jb}}{Q_b} - \frac{N_{jd}}{Q_d}\right) A_b \, dz + V(1 - \delta)(1 - \varepsilon_{mf})\rho_p r_j \qquad (7)$$

Using equation (2) the integral of equation (7) is evaluated and equation (7) becomes:

$$(N_j)_d = y_{jF} N_F \frac{Q_{dF}}{Q_F} + U_b A_b \left(\frac{y_{jF} N_F}{Q} - \frac{(N_j)_d}{Q_d}\right) + \left(1 - e^{-a_j.H}\right) + V(1 - \delta)(1 - \varepsilon_{mf})\rho_p r_j \qquad (8)$$

The total moles of component j leaving the reactor are given by:

$$N_j = (N_j)_d + (N_j)_b \qquad (9)$$

Similarly we obtain the following expression for the energy balance around the dense phase for adiabatic operation:

$$\rho_g C_{pg} Q_{dF} (T_F - 298) - \rho_g C_{pg} Q_d (T_d - 298) + \rho_g C_{pg} U_b A_b (T_F - T_d)\left(1 - e^{-b.H}\right) + V(1 - \delta)(1 - \varepsilon_{mf})\rho_p (-\Delta H_r) r_j = 0 \qquad (10)$$

The fluidized bed exit temperature is given by:

$$T_{exit} = \frac{Q_b T_b + Q_d T_d}{Q_b + Q_d} \qquad (11)$$

6. The Reaction Kinetics

The stoichiometric equation for the ammonia synthesis has the form:

$$3H_2 + N_2 \rightleftharpoons 2NH_3 \qquad \Delta H = -92.44 \text{ kJ/mol}$$

In this model the intrinsic modified form of the Temin rate expression is used:

$$r_{NH_3} = k_2 \left[k_a^2 f_{N_2} \left(\frac{f_{H_2}^3}{f_{NH_3}^2}\right)^{\alpha} - \left(\frac{f_{NH_3}^2}{f_{H_2}^3}\right)^{1-\alpha}\right] \qquad (12)$$

r_{NH_3} is the reaction rate in kmol of NH3/(h.m3 of the catalyst bed), K2 is the velocity constant for the reverse reaction in kmol /(h.m3) and Ka is the equilibrium constant of the reaction.

The velocity constant is estimated by the Arrhenius relation of the form:

$$K_2 = K_{20} \exp\left(-\frac{E_2}{R.T}\right) \qquad (13)$$

The respective values for the Montecatini Edison catalyst are:

$$\alpha = 0.55, \qquad E_2 = 1.635 \times 10^5 \frac{kJ}{Kmol}$$

$$\text{and} \qquad \log_{10} K_{20} = 14.7102$$

The equilibrium constant is given by Gaines

$$\log K_a = -2.691122 \log T - 5.519265 \times 10^{-5} T + 1.848863 \times 10^{-7} T^2 + \frac{2001.6}{T} + 2.6899 \qquad (14)$$

The fugacity of component is given by definition as:

$$f_j = \varphi_j x_j P \quad (15)$$

Where:

φ_j is the fugacity coefficient of component j

x_j is the mole fraction of component j

P is the total pressure in atm

7. The result of ammonia modeling in fluidized bed reactor

It can be noticed from figure (4) the conversion is increases gradually by almost constant rate along the bed, the advantage of mass transfer between the bubble and emulsion phase and that the reaction occurs just in the emulsion phase don't allow the concentration of ammonia in the reaction zone to increase and so reduce the rate of the reversible reaction and producing nitrogen. Also the good mixing of the fluidized bedcontribute on the temperature control and hence the rate of reaction, so the curve is almost a line.

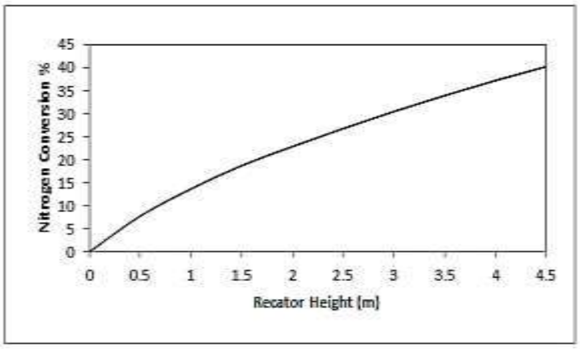

Fig 4: Change of Nitrogen Conversion along the Reactor

7.1 Mole Fraction of the components along the Reactor

The mole fraction of nitrogen, hydrogen, and ammonia is also calculated from the initial amount of the component and the conversion of nitrogen and illustrated in figure (5) below.

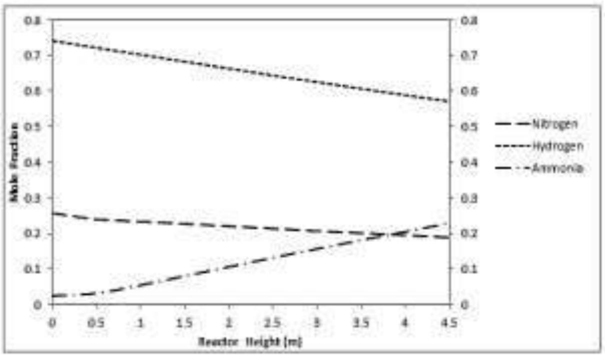

Fig 5: Change of component mole fraction along the Reactor

7.2 The Effect of Catalyst Particle Size on the Conversion

Figure (6) below conclude the tests done accounting for catalyst particle size. Fixed bed use large sizes of catalyst particles (6 – 12 mm) to avoid excessive pressure drops in the reactor [8]. The smaller sizes of particles in fluidized beds eliminate pore diffusion limitations associated with the use of larger particles and hence contribute in increasing the conversion.

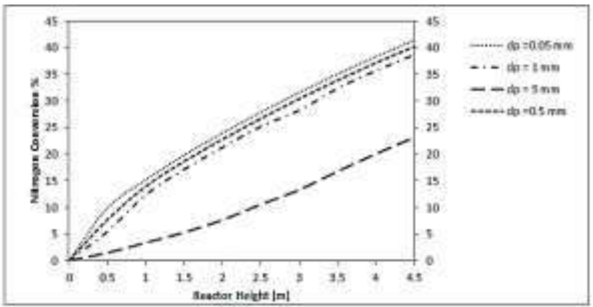

Fig 6: The effect of Particle Diameter on Conversion along the Reactor

7.3 Effect of mass transfer between the bubble and dense phases

It is well known that mixing tends to increase the conversion [9]. Also, the bypass of a certain percentage to reactants through the bubble phase has negative effect on the conversion in fluidized bed reactors.

Mass transfer between phases enhances the conversion of the forward reaction for the reversible reactions, the ammonia which transfer to the bubble phase cannot convert to nitrogen because the reaction occurs only in the dense phase. Figure (7) shows that the conversion obtained when components allow to transfer between beds (Kbd≠0) the conversion is 40.26%which is high percentage while when the mass transfer coefficient is set to 0 the conversion is only 31.36%. It can be concluded that the net effect of mass transfer between phases results in increasing the conversion.

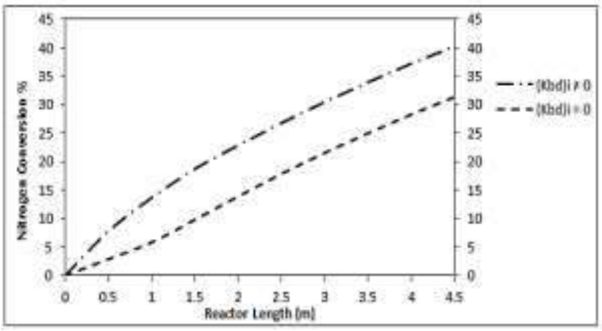

Fig 7: The effect of components mass transfer between Phases

7.4 The Effect of Bed Height to Diameter

Figure (8) shows the effect of the height to diameter ratio on the nitrogen conversion. It 1s clear that this parameter has considerable effect on the conversion. The increase of the height to diameter ratio (by decreasing the bed diameter while keeping the total volume constant) decreases the gas flow in the emulsion phase, thereby increasing the bubble gas flow as shown in Figure (9). Since the reaction occurs mostly in the emulsion phase. The decrease of the gas flow has a negative impact on the conversion. Also, the increase of the bubble gas flow affects the conversion negatively [11]:

- By increasing bubble by passing.
- By increasing the bubble size, increase the bubble velocity, decrease the residence time, and decrease the overall coefficient of the gas transfer between the bubble and emulsion phases.

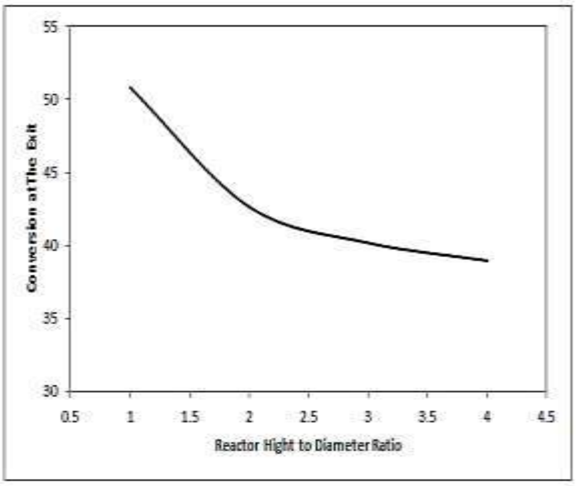

Fig 8: Effect of Bed Height to Diameter Ratio on the Conversion

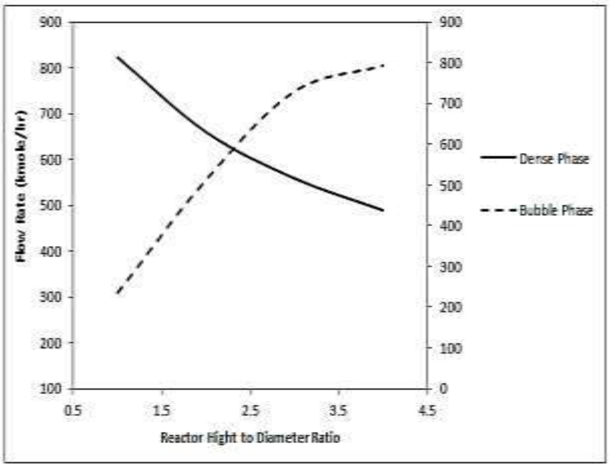

Fig 9: Gas Flow in the Bubble and Dense Phases

8. Conclusions

In the production of ammonia in the fixed bed reactors, the nitrogen conversion was 26.76% while in the fluidized bed reactors, the conversion increased to 40.26% at the end of the reactor, which reflected positively on the amount of ammonia produced.

The effect of some factors on the performance of the reactor, such as pressure and temperature, the particle size and the ratio of the reactor diameter to high were also investigated. The most important factor affecting the production is the mass transfer between dense and bubble phase. Where the conversion of nitrogen when salted by the mass transfer of material, which actually happens 40.26%, but when the mass transfer coefficients of materials adjusted to zero the conversion of nitrogen decline to 31.36%.

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