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Modeling and Simulation of Methanol Synthesis in Fluidized Bed Reactor

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Abstract— *In this pater a fluidized bed reactor for methanol reaction 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 methanol production rate. The results have been compared with the available industrial data; the comparison shows that there is 30% increase in methanol flow rate when produce in fluidized bed reactor.*

Keywords— *Fluidized bed reactor, Methanol, Two phase model.*

I. INTRODUCTION

The annual production of methanol exceeds 40 million tons and continues to grow by 4% per year. Methanol has traditionally been used as feed for production of a range of chemicals including acetic acid and formaldehyde. In recent years methanol has also been used for other markets such as production of DME (Di-methyl-ether) and olefins by the so-called methanol-to-olefins process (MTO) or as blend stock for motor fuels [1].

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

II. MODELING OF FLUIDIZED BED REACTOR

The fluidized-bed reactor has the ability to process large volumes of fluid [2]. 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 1.

III. DESCRIPTIVE BEHAVIOR OF 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. 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.

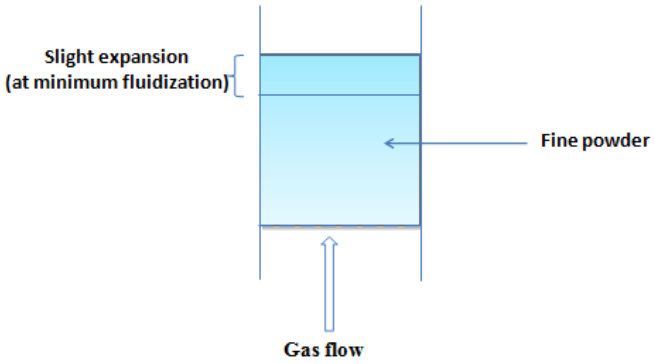

Fig. 1. Fine powder inside a tube starting to fluidize due to gas flow rate

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 [3]. 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".

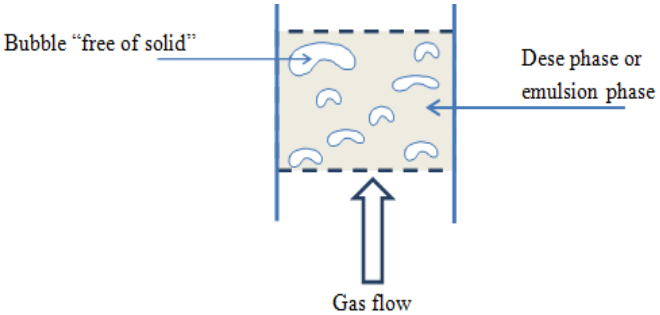

Fig. 2. Phases of fluidized bed [11].

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IV. Model Assumptions

The mathematical model is developed based on the two phase reactor model. The following assumptions are used to simplify the model equations [4]:

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

V. General Model Formulation

Based on the two-phase model, a fluidized catalytic bed reactor can be divided into two regions; 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 [9].

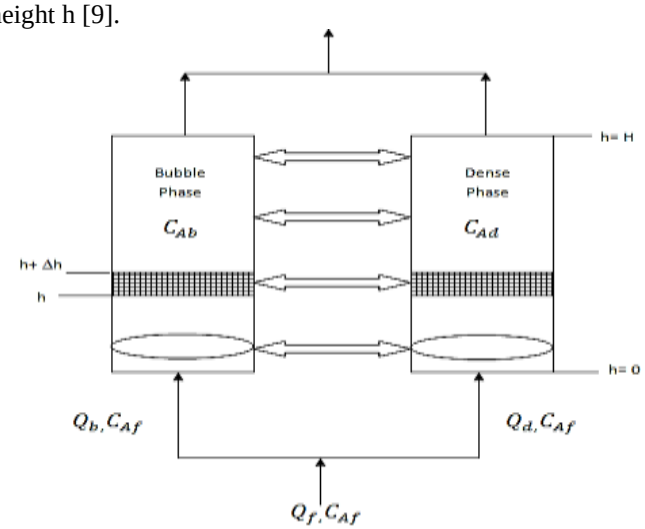

Fig. 3. The two phases of fluidized bed.

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*

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 [10]

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

With the initial conditions $N_{jb} = N_{jbF} \quad at\ z = 0$. 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:

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

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

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:

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

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 [5]:

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

The fluidized bed exit temperature is given by:

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

VI. The Reaction Kinetics

The reactions together with the water-gas shift reaction are:

$CO + 2H_2 \rightleftharpoons CH_3OH \qquad \Delta H^{\circ}_{298} = -90.55\ kJ.mol^{-1}$

$CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O \qquad \Delta H^{\circ}_{298} = -49.43\ kJ.mol^{-1}$

$CO_2 + H_2 \rightleftharpoons CO + H_2O \qquad \Delta H^{\circ}_{298} = 41.12\ kJ.mol^{-1}$

In this study, the kinetic equation proposed by Vanden Bussche and Froment is used [6]. The equation is based on equation (2) and (3) and thus the reaction rate r 1 is neglected. The kinetic equation is:

$$r_{CH_3OH} = \frac{k_1 P_{CO_2} P_{H_2} \left(1 - \frac{P_{CH_3OH} P_{H_2O}}{K_2^{eq} P_{CO_2} P_{H_2}^3}\right)}{\left(1 + \frac{k_3 P_{H_2O}}{P_{H_2}} + \sqrt{k_4 P_{H_2}} + k_5 P_{H_2O}\right)^3} \qquad (12)$$

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$$r_{RWGS} = \frac{k_2 P_{CO_2}\left[1 - K_3^{eq}\left(\frac{P_{H_2O}P_{CO}}{P_{CO_2}P_{H_2}}\right)\right]}{\left(1 + \frac{k_3 P_{H_2O}}{P_{H_2}} + \sqrt{k_4 P_{H_2}} + k_5 P_{H_2O}\right)} \quad (13)$$

VII. The Result of Methanol Modeling in Fluidized Bed Reactor

A two phase model of fluidized bed reactor has been generated for methanol convertor. Figure (4) shows the flow rate of the main component in the reaction, it will be noticed that the production of methanol is increase by 30% for the same conditions as compared with the production in the fixed bed reactor.

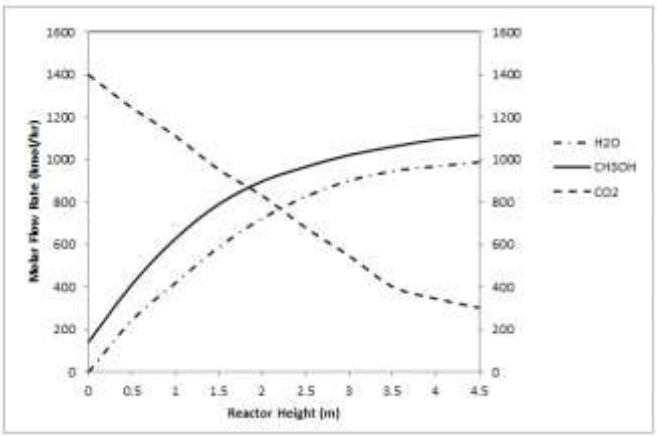

Fig. 4. Methanol flow rate along fluidized bed reactor.

Conversion of CO_2 and H_2 along the reactor
The conversion is also improved from the fixed bed; the conversion of carbon dioxide at the exit of the fluidized bed is 75% against 51% for the fixed bed.

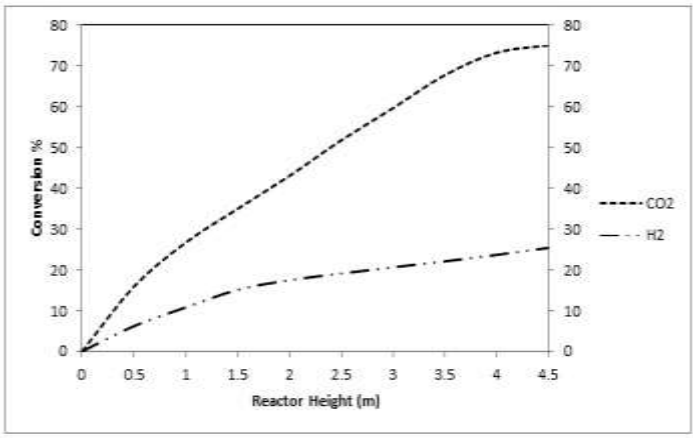

Fig. 5. The change of conversion along the reactor.

The effect of catalyst particle size on the conversion
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 methanol production [8]; figure (6) shows the flow rate of methanol for different particle size.

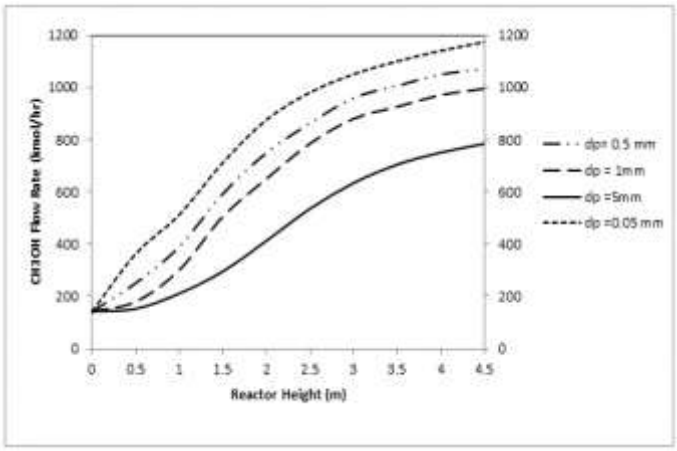

Fig. 6. Effect of particle size on the methanol production.

Effect of mass transfer between the bubble and dense phases
Mass transfer between phases improves the methanol production flow rate. Figure (7) shows that there is 40% increase in methanol flow rate with mass transfer between phases.

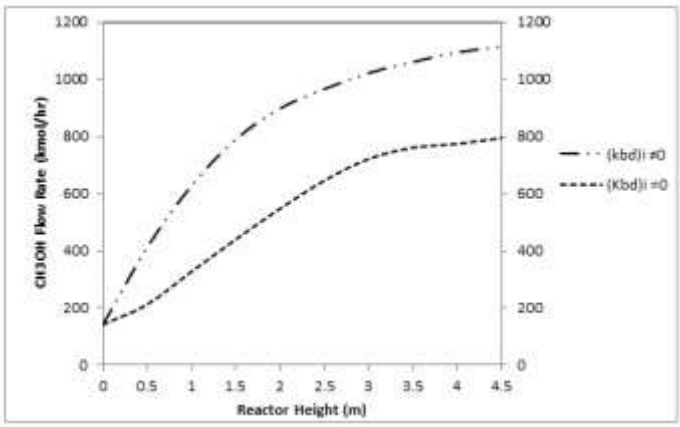

Fig. 7. The effect of mass transfer on methanol production.

The Effect of Bed Height to Diameter
The effect of the reactor dimensions is illustrated in figure (8) below, 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 [7]:

- 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.

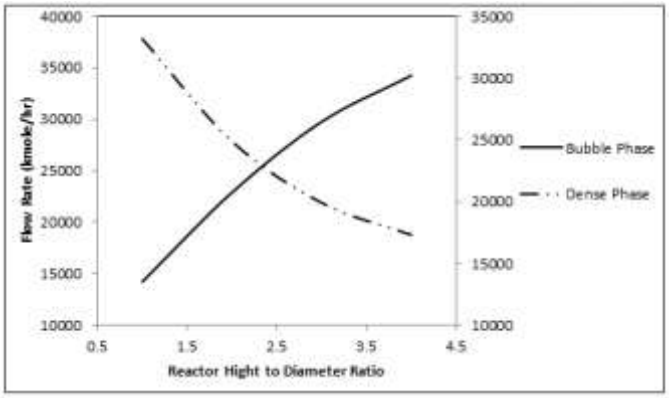

Fig. 8. The effect of height to diameter ratio on phases flow rate.

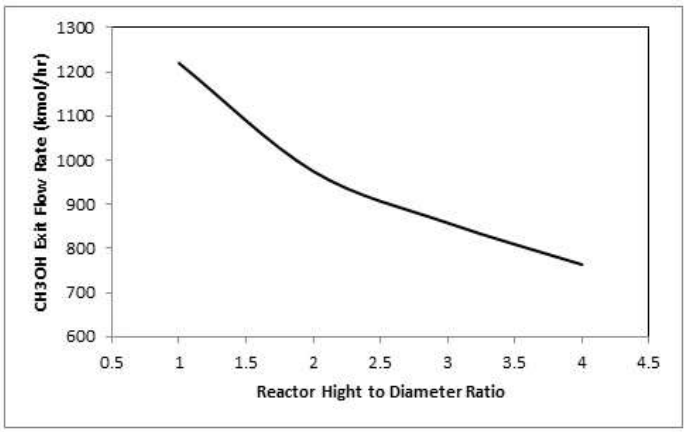

Fig. 9. The effect of height to diameter ratio on methanol production.

The Effect of Initial Pressure

The flow rate of methanol is tested for different values of initial gas pressure figure (10) shows that the production is improved by increasing the pressure.

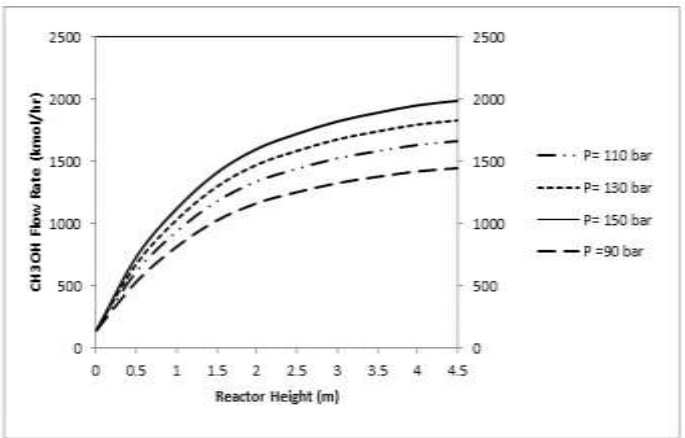

Fig. 10. The effect of initial pressure on methanol flow rate.

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