

APPROCH TO MODELLING OF GAS-SOLID FLUIDIZED BED REACTOR

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Received September 22, 2005; received in revised form March 20, 2006, accepted June 24, 2006

ABSTRACT

During the past few decades, numerous contributions and advances have been accomplished in the field of fluidization. Despite these continuous efforts there has not been much success in setting up a strongly reliable model for the design of catalytic fluidized bed reactors, fluidized bed reactors are usually modeled as a multiphase system consisting of two or three distinct phases. The two-phase theory of fluidization was originally proposed by Toomey and Johnstone (1952) this theory considers a gas-fluidized bed to be composed of two phases a dense or emulsion phase consisting of solid particles and Interstitial gas and a dilute or bubble phase consisting of rising void essentially free from particles. The three-phase theory of fluidization was originally proposed by Kunii and Levenspiel(1968)^[11] they proposed the bubbling bed model (for gas-solid system) which considers the cloud-wake region as a separate phase In addition to the emulsion and bubble phase. In the multistage three-phase model (El- Halwagi and El-Rifai (1988)^[4]) considered that the fluid bed to be composed of a number of equivalent stages in series. Within each stage exchange of gas takes place between the bubbles cloud-wake and emulsion phase. The mathematical equations (linear finite difference equations) of multistage three-phase model with first order reaction analytically solved and the concentration profile along the bed has been obtained.

The mathematical equations of two – phase model (Werther (1980-1992)^[17] with nth order reaction solved by Runge Kutta method and the concentration profile along the bed has been obtained. The results of concentration profile for the two models are being compared and finally model results are being compared with experimental results from the literature.

Key words: fluidized bed, mathematical, modelling, mas, solid

1. Introduction

Fluidized bed reactors are usually modeled as a multiphase system consisting of two or three distinct phases .The two-phase theory of fluidization was originally proposed by Toomey and Johnstone ^[15]. This theory considers a gas-fluidized bed to be composed of two phases; a dense or emulsion phase consisting of solid particles and interstitial gas and a dilute or bubble phase consisting of rising voids essentially free from particles. It also assumes that all the gas in excess of the minimum – fluidization flow rate passes through the bed as bubbles. The emulsion phase is considered to be similar to the bed under incipient – fluidization conditions.

Based on the two - phase theory, various models have been proposed ^[9,16,18,19,20,21,22,23,24,25,26]

These models differ substantially in the assumptions they suggest regarding the flow behavior of each phase, the extent of gas mixing and the mode of interphase gas transfer.

Kunii and Levenspiel^[11] proposed the bubbling – bed model which considers the cloud – wake region as a separate phase, in addition to the emulsion and bubble phases, bulk flow of gas through the emulsion and cloud – wake phases is assumed to be negligibly small.

Comparative studies reviewing the different models of fluidized – bed reactors may be found in the literature^[2,3,7,8,27,28,21,29,30,31,32].

Although these models have contributed considerably in establishing many fundamental concepts of fluidized – bed reactors none of them has proved to be of wide and reliable applicability. Thus it seems necessary to introduce more fluidized – bed models which take account of the basic underlying physics of fluidization. This work has been undertaken in an attempt to show a novel model that would reasonably reflect the real performance of gas - solid fluidized bed catalytic reactors. This model will be referred to as the “multistage three – phase model”^[9,4]. It is based upon a realistic but rather simple visualization of the basic hydrodynamic aspects of fluid beds. The assumption of first – order kinetics in the proposed model made it possible to obtain an exact analytical solution for the concentration profiles along the bed.

Simultaneously with that multistage three – phase model, the two – phase model^[16,17] with any reaction order, will be used to modelling the gas – solid fluidized bed reactor. Experimental data available in the literature on first – order catalytic reactions in gas – solid fluidized beds were used to assess the validity of the multistage three – phase and two – phase models.

1.1) TWO – PHASE MODEL^[16,17,13]

The mass balances on the reactor volume elements $\Delta t \times dh$ for a species i in the bubble and suspension phases respectively are in the case of a heterogeneously catalyzed reactor:

$$\epsilon b \frac{\partial C_{bi}}{\partial t} = -(U - Umf(1 - \epsilon b)) \frac{\partial C_{bi}}{\partial h} - k_{GI} at(C_{bi} - C_{di}) \quad (1)$$

$$(1 - \epsilon b)(\epsilon mf + (1 - \epsilon mf)\epsilon i) \frac{\partial C_{di}}{\partial t} = -Umf(1 - \epsilon b) \frac{\partial C_{di}}{\partial h} + k_{GI} at(C_{bi} - C_{di}) + (1 - \epsilon b)\rho_s \sum_{J=1}^M v_{IJ} r_J \quad (2)$$

For Steady state condition and reactant i with reaction rate ($r_i = km.cd^n$), $km = \frac{k}{\rho_s(1 - \epsilon mf)}$

The equation will be as below:

$$\frac{\partial C_{bi}}{\partial h} = \frac{-k_{GI} at}{(U - Umf(1 - \epsilon b))} (C_{bi} - C_{di}) \quad (3)$$

$$\frac{\partial C_{di}}{\partial h} = \frac{k_{GI} at}{Umf(1 - \epsilon b)} (C_{bi} - C_{di}) + (1 - \epsilon b)\rho_s \sum_{J=1}^M v_{IJ} r_J \quad (4)$$

at $h=0$, $C_{bi}=C_o$ and $C_{di}=C_o$

So the above equation will be solved by Runge Kutta fourth order methods , The solved results will be as:

$$C_{bi}(h) = C_{bi(0)} + 1/6(K_1 + 2K_2 + 2K_3 + K_4) \quad (5)$$

$$C_{di}(h) = C_{di(0)} + 1/6(L_1 + 2L_2 + 2L_3 + L_4) \quad (6)$$

with that above equations, the concentration profile along bed will be obtained.

The overall fractional conversion and average gas concentration are given by:

$$x=1-\frac{\bar{C}}{C_0}, \quad \bar{C}=(U_b * C_b + U_{mf} * C_d) / U \tag{7}$$

1.2) MULTISTAGE THREE-PHASE MODEL [4,9,14]

Figure 1 shows a schematic representation of the basic features of the proposed model.

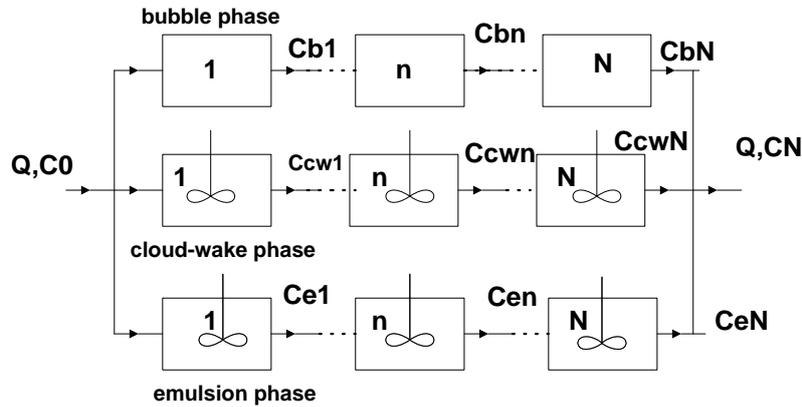


FIG1: Multistage three-phase model

Material balance equations for reactant gas around stage n for each of three phases are as follows:

Bubble phase:

$$U_b C_{bn-1} - U_b C_{bn} - (K_{bc})_b \epsilon b \int_{z_{n-1}}^{z_n} (C_b - C_{cwn}) dz = 0 \tag{8}$$

Cloude – wake phase:

$$U_{cw} C_{cwn-1} + (K_{bc}) b \epsilon b \int_{z_{n-1}}^{z_n} (C_b - C_{cwn}) dz + K_{ce} C_{en} - (U_{cw} + k_{cw} + K_{ce}) C_{cwn} = 0 \tag{9}$$

where :

$$K_{ce} = (K_{ce}) b \epsilon b \Delta z \tag{10}$$

$$\text{and } k_{cw} = k_{fcw} \times \epsilon b \Delta z \tag{11}$$

in which k is the reaction rate constant based on the unit volume of the dense phase (emulsion phase and cloud – wake phase) and according to the first assumption of the model:

$$\Delta z = z_n - z_{n-1} = Db \tag{12}$$

Emulsion phase:

$$U_{mf} C_{en-1} + K_{ce} C_{cwn} - (U_{mf} + k_e + K_{ce}) C_{en} = 0 \tag{13}$$

Where:

$$k_e = k[1 - \epsilon b(1 + f_{cw})] \Delta z \tag{14}$$

The material balance on reactant gas over the differential element of height in the bubble phase is written as:

$$U C_b - U_b (C_b + dC_b) - (K_{bc})_b (C_b - C_{cwn}) dz = 0 \tag{15}$$

Which may be rearranged and integrated to give

$$\int_{Cb_{n-1}}^{Cb} \frac{dCb}{Cb - Ccwn} = \frac{-(Kbc)_b \epsilon b}{Ub} \int_{z_{n-1}}^z dz \quad (16)$$

$$Cb - Ccwn = (Cb_{n-1} - Ccwn) \exp\left[-\frac{(kbc)_b \epsilon b (z - z_{n-1})}{Ub}\right] \quad (17)$$

At the bottom of the bed ($n=0$) the concentration of gas fed to each phase is the same as that of the incoming feed gas. Hence the appropriate boundary condition are:

$$\text{At } n=0 \quad C_{bn}=C_{cwn}=C_{en}=C_0 \quad (18)$$

Equations (8),(9),(13) C_n and (17) may be solved analytically to give the reactant gas concentration of each phase Leaving any stage n ($1 \leq n \leq N$) as

$$Cbn = f_1 GL_1^n + f_2 GL_2^n + f_3 GL_3^n \quad (19)$$

$$Ccwn = gs_1 f_1 GL_1^n + gs_2 f_2 GL_2^n + gs_3 f_3 GL_3^n \quad (20)$$

$$Cen = rs_1 f_1 GL_1^n + rs_2 f_2 GL_2^n + rs_3 f_3 GL_3^n \quad (21)$$

were the parameters $f_1, f_2, f_3, g_{s1}, g_{s2}, g_{s3}, GL_1, GL_2, GL_3, r_{s1}, r_{s2}$ and r_{s3} may be calculated from relations.

The average gas concentration of reactant Leaving the n^{th} stage \bar{C}_n , is defined as the concentration that one would measure by sampling the gas leaving stage in proportion to the volumetric flow rates of the three phases:

$$\bar{C}_n = (U_b C_{bn} + U_{cw} C_{cwn} + U_{mf} C_{en}) / U \quad (22)$$

Therefore, the gas concentration profiles for the three phases and for the average concentration may be obtained from equations (19),(20),(21) and (22) respectively, and the outlet gas concentration \bar{C}_N is calculated directly by substituting for $n=N$ in eq (22). The overall fractional conversion is given

$$\text{by } x=1 - \frac{\bar{C}_N}{C_0} \quad (23)$$

2- BASIC ASSUMPTION AND PARAMETERS OF THE MODELS

The multistage three-phase model assumptions and parameters consists of (bubble diameter, bubble velocity, bubble volume,..) refers to [4,13]. The two- phase model assumptions and parameters refers to [7,8,16,17].

3 – RESULTS AND DISCUSSION

In this section by comparing models results with published experimental data on the conversions and concentration profiles of first-order isothermal catalytic reaction carried out in gas-fluidized beds, the predictive power of the proposed models are evaluated.

(3.1) Lewis et al. [12] studied on the ethylene hydrogenation reaction in a fluidized bed with 0.075 m diameter. The comparison between the experimental conversion values obtained by Lewis et al and the two & three phase models have been shown in Fig. (2). Results show a better match between the two - phase model and the experimental values, where as three phase model has pronounced deflections at higher velocities which could also be due to the small reactor diameter.

(3-2) Ozone Decomposition

Kobayashi et al.^[10] studied on the ozone decomposition reaction in a 0.083 m diameter reactor. Figure (3) shows the comparison between the experimental conversion values obtained by Kobayashi et al.^[10] and the two & three phase models.

Results show that the experimental conversion values do not match with three - phase model. this deflection could be due to the small reactor diameter ($D_r=0.083\text{m}$) and also due to the small reaction rate constant ($k=0.75 \text{ sec}^{-1}$).

Freyer and Potter^[4,5] studied on the ozone decomposition reaction in a 0.229 m diameter reactor. Figure (4) shows the comparison between the experimental conversion factors and the two & three phase models. it can be seen a better match between the experimental results and the two, & three phase models. This is mainly due to the right selection of the reactor diameter and reaction rate ($D_r= 0.229 \text{ m}$, $k= 3.60 \text{ sec}^{-1}$).

Outlet / inlet concentration ratio obtained from the two & three phase models has been compared with the experimental values and results have been shown in figures 5P2, 5P3, 6P2, and 6P3. It can be seen that the two - phase model have a better match with the experimental values (figure 5P2, 6P2). Only small deflection occurs at medium range velocities ($0.05 < U < 0.1 \text{ m/sec}$). There is a good match between the three - phase model and the experimental values (Fig., 5P3), but a mismatch in Fig. 6P3 is mainly due to the small reaction rate constants ($k=0.33 \text{ sec}^{-1}$). Figures 7P2 and 7P3 showing the plots of conversion factor, bubble, dense, cloud - wake, emulsion phases and outlet concentrations versus reactor bed height. It can be seen that the shape of profiles are as expected.

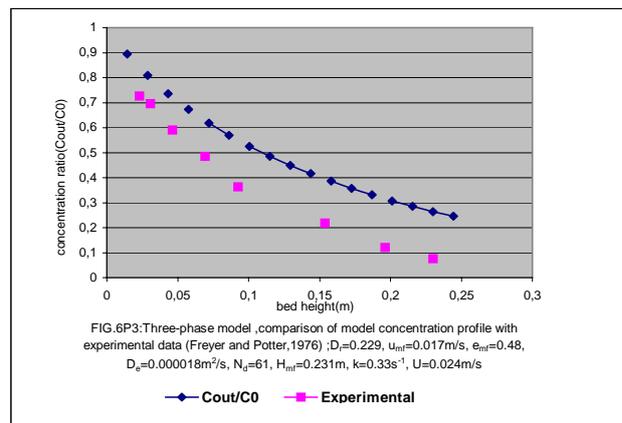
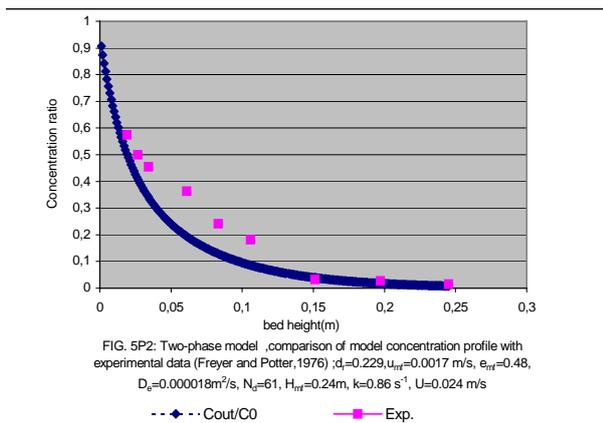
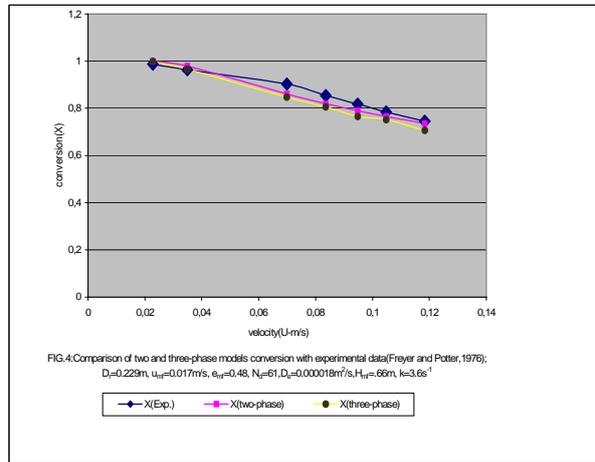
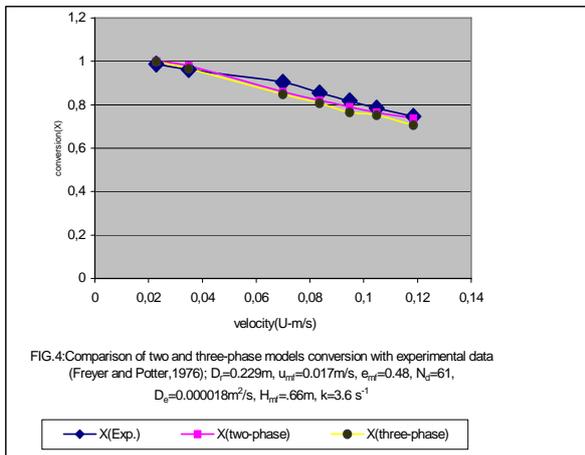
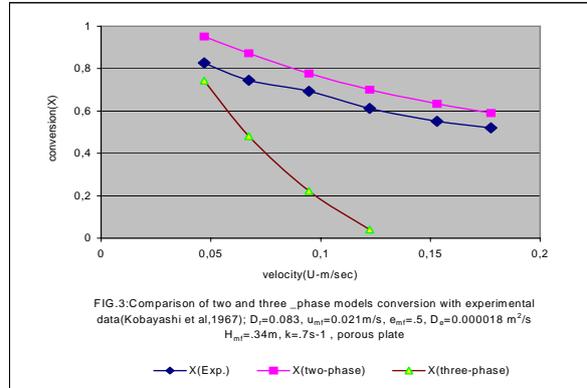
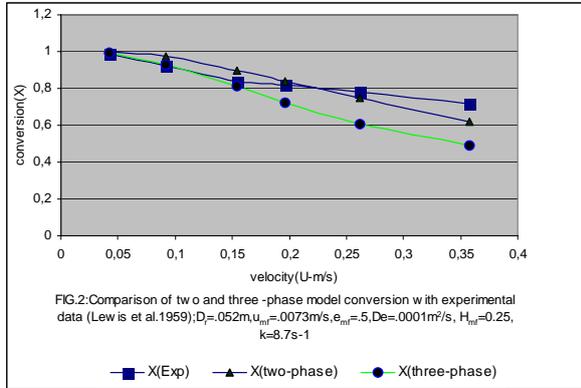
Bauer et al.^[1,17] studied on the ozone decomposition reaction in a 0.083 m and 1 m diameter reactors. The comparison between the experimental conversion values obtained by Bauer et al. (versus reaction rate constant, k) and two - phase model have shown in figures 8P2 and 9P2. Results show (Fig. 8P2) a better match between the two phase model and the experimental values, whereas the results of pilot scale reactor (Fig. 9P2) show deflection with experimental data. This shows that model parameters equations do not predict correct value for model parameters and therefore right equations should be replaced. Three-phase model due to small reaction rate values can not predict correct value for conversion..

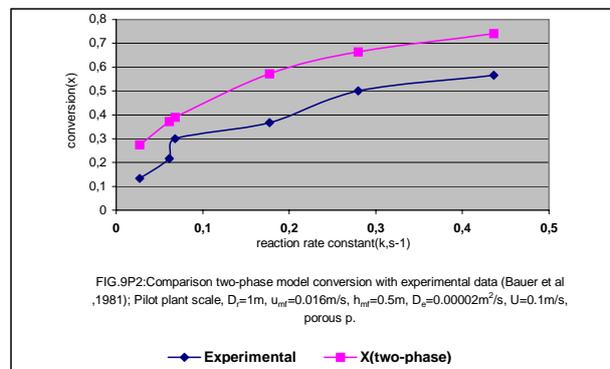
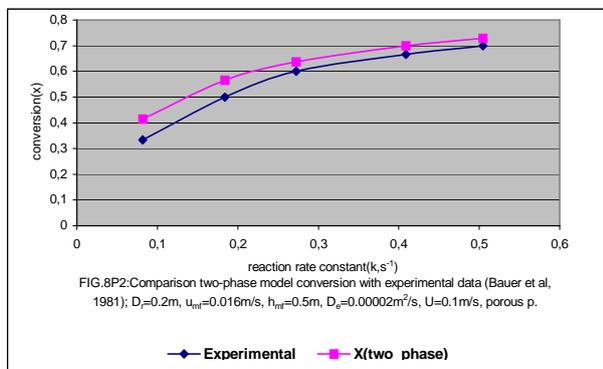
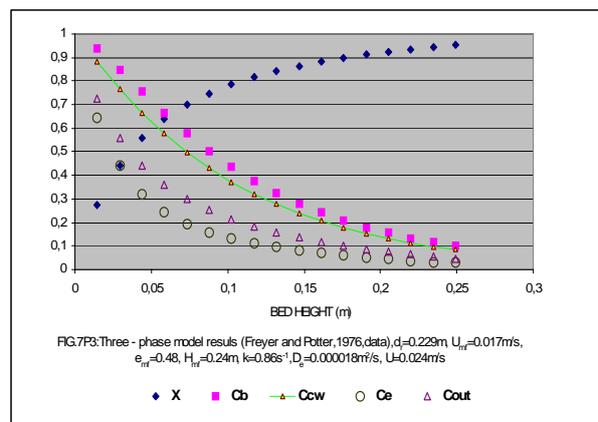
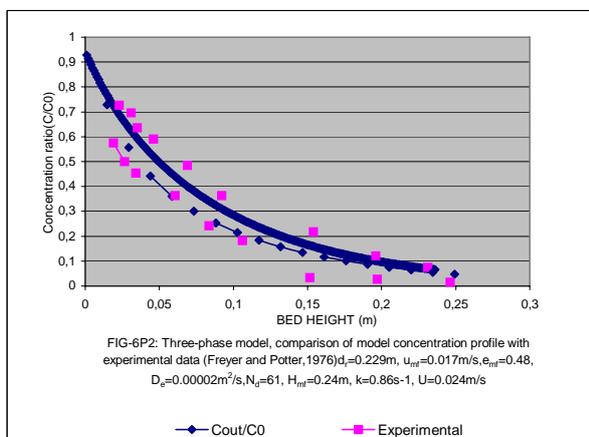
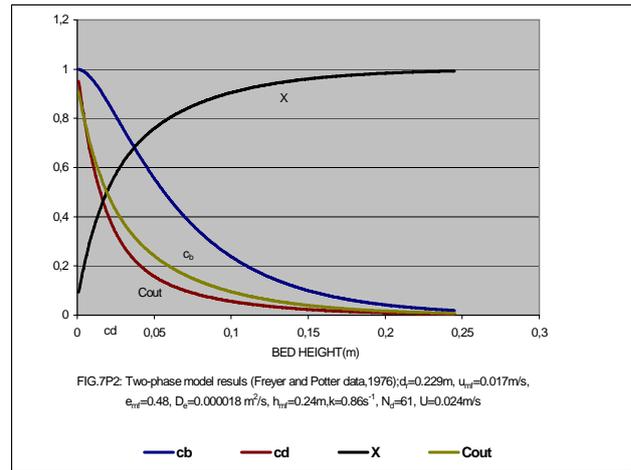
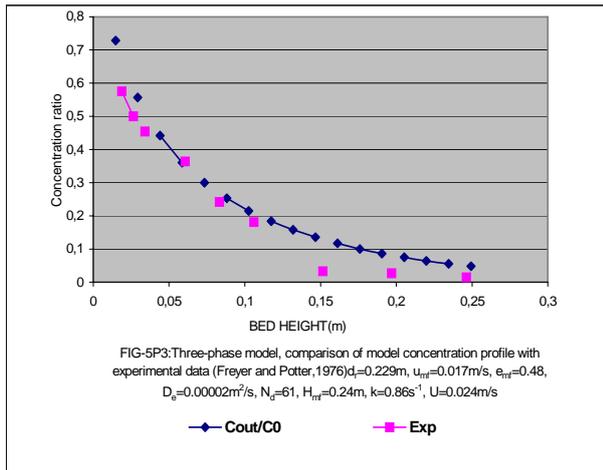
4- CONCLUSION

1. Three – phase multistage model and two-phase model have been developed respectively for the first & nth order reactions in a fluidized bed gas-solid reactor.
2. The multistage three – phase model is much more complicated compare to the two-phase model hence, mathematical equations for the three – phase model need to be solved with special analytical & numerical methods.
3. For the bench scale fluidized bed reactor ($D_r < 0.1\text{m}$) and rate constants less than $1.0 (K < 1\text{sec}^{-1})$, results of the multistage three – phase model do not match well with the experimental data on the contrary there is a good match between the two-phase model results and the experimental data. the mismatch between the three – phase model and the experimental results is due to the sensitivity of the model to the rate constant values. This sensitivity is more pronounced at rate constants less than 1.0 , which model can not predict actual conversion values.
4. For the pilot scale fluidized bed reactor ($D_r=1\text{m}$) results of the two – phase model and the experimental data fairly match each other (Fig. 9P2). Therefore due to the simplicity in two-phase

model and good match with the experimental data it is advised to be used prior to any other more complicated models.

Figures:





NOTATION

- a_t volume specific mass transfer area between bubble and suspension phase, m^{-1}
- C_b concentration in bubble phase, $kmole/m^3$
- C_{bn} gas concentration of reactant leaving stage n of bubble phase, $kmole/m^3$
- C_{cwn} gas concentration of reactant leaving stage n of cloud-wake phase, $kmole/m^3$
- C_{en} gas concentration of reactant leaving stage n of emulsion phase, $kmole/m^3$
- C_d gas concentration of reactant Dense (emulsion) phase, $kmole/m^3$
- C_0 initial gas concentration of reactant, $kmole/m^3$
- \bar{C} average gas concentration of reactant leaving reactor, $kmole/m^3$

\bar{C}_n	average gas concentration of reactant leaving stage n, kmole/m ³
D_b	average equivalent bubble diameter, m
D_e	gas phase diffusion coefficient, m ² /sec
D_r	bed diameter, m
f_{cw}	ratio of cloud-wake volume to bubble volume.
f_1, f_2, f_3	the parameters of mathematical solution in three-phase model.
GL_1, GL_2, GL_3	the parameters of mathematical solution in three-phase model.
g_{s1}, g_{s2}, g_{s3}	the parameters of mathematical solution in three – phase model.
h	height above distributor level, m
h_1	height interval of Runge Kutta methods.
H_{mf}	bed height under minimum fluidization condition, m
K_1, K_2, K_3, K_4	constants parameters in Runge Kutta methods.
k	reaction rate constant based on unit volume of dense phase, s ⁻¹
km	reaction rate constant based on unit weight of catalyst, m ³ /(kg.s)
k_{cw}	constant defined in eq. (11) m/s
K_{ce}	constant defined in eq. (10) m/s
k_e	constant defined in eq. (14) m/s
$(K_{bc})_b$	volumetric rate of gas exchange between bubble and cloud – wake phases, s ⁻¹
$(K_{ce})_b$	volumetric rate of gas exchange between cloud – wake and phases, s ⁻¹
k_G	mass transfer coefficient of gas component, m/s
L_1, L_2, L_3, L_4	constants parameters in Runge Kutta method
n_r	reaction order
N	total number of stages in bed.
N_d	number of orifice openings on the distributor.
r_{s1}, r_{s2}, r_{s3}	the parameters of mathematical solution in three – phase model.
t	time, s
U	superficial velocity of fluidization, gas, m/s
U_b	superficial gas velocity of bubble phase, m/s
U_{cw}	superficial gas velocity of cloud-wake phase, m/s
U_{mf}	superficial velocity of fluidization gas under minimum fluidization condition, m/s
x	fractional conversion of reactant gas leaving the bed.
z	height above gas distributors, m

GREEK LETTERS

Δz	stage height, m
ϵ_b	volume fraction of bubbles in the bed
ϵ_{mf}	mean voidage under minimum – fluidization condition.
V_{ij}	stoichiometric number of species i in reaction j.

SUBSCRIPTS

b	bubble phase
c_w	cloud-wake phase
e	emulsion phase
n	stage number
N	final stage

REFERENCES

- [1] Bauer, W., Werther, J. and Emig, G., Ger. Chem. Eng. 4, 291-298., 1981
- [2] Bukur, D.B. and Nasif, N.: The Effect of Bubble Size Variation on the Performance of Fluidized Bed Reactors. Chem. Eng. Sci. 40, 1925-1933. 1985
- [3] Bukur, D.B., Nasif, N. and Daly, J.G., On the Use of Effective Bubble Diameters in the Counter Current Back Mixing Model for Fluid Bed Reactors. Chem. Eng. Sci. 42, 1510-1513, 1987
- [4] El-Halwagi, M.M. and El-Rifai, M.A., Mathematical Modeling of Catalytic Fluidized Bed Reactors- the Multistage Three – phase Model, Chem. Eng. Sci. 44(9), 2477-2486, 1988
- [5] Freyer, C. and Potter, O.E., Experimental Investigation of Models for Fluidized Bed Catalytic Reactors, AIChE Journal, 22(1)38-47, 1976
- [6] Freyer, C. and Potter, O.E., Counter Current Back Mixing Model for Fluidized Bed Catalytic Reactors. Applicability of Simplified Solutions. Ind. Eng. Chem. Fundam, 11, 338-344, 1972
- [7] Grace, J.R. and Sun, G., Powder Technology 62, 203-205, 1990
- [8] Grace, J.R. and Sun, G., Can.J.Chem. Eng. 69, 203-205, 1961
- [9] Kato, K. and Wen, C.Y., Bubble assemblage model for kinetic process in fluidized bed. Ind. Eng. Chem. Process Des. Dev. 7, 481-492, 1969
- [10] Kobayashi, H., Arai, F., Izawa, N. and Miya, T., 1967. Chem. Eng. Japan, 5, 28-32, 1967
- [11] Kunii, D. and Levenspiel, O., Fluidization Engineering, John Wiley New York, 1992
- [12] Lewis, W.K., Gilliland, E., R. and Glass, W., Solid Catalyzed Reaction in a Fluidized Bed, A.I.C.h.E.J, 5, 419-429, 1959
- [13] Mori, S. and Wen, C.Y. Estimation of Bubble Diameter in Gaseous Fluidized Beds, A.I.Ch.E.J, 21, 109-115, 1975
- [14] Peters, M.H., Fan, L.S. and Sweeney, T.L., Reactant Dynamic in Catalytic Fluidized Bed Reactors with Flow Reversal of Gas in the Emulsion Phase. Chem. Eng. Sci. 37, (4-6), 553-565, 1982
- [15] Toomey, R.D. and Johnstone, H.F., Gaseous Fluidization of Solid Particles. Chem. Eng. Prog. 48, 220-226, 1952
- [16] Werther, J., Mathematical Modelling of Fluidized Bed Reactors, Int. Chem. Eng 20, 529-541, 1980
- [17] Werther, J., Scale up Modelling for Fluidized Bed Reactors, Chem. Eng. Sci., 47, no.9-11, 2457-2462, 1992
- [18] Davidson J.F. and D. Harrison D., *Fluidized Particles*, Cambridge University Press, London, 1963.
- [19] Partridge, B. A., Rowe, P. N., *Trans. Inst. Chem. Eng.*, 44, 349 (1966)
- [20] Kato, K.; Wen, C. Y. Bubble Assemblage Model for Fluidized-Bed Catalytic Reactors. *Chem. Eng. Sci.*, 24, 1351, 1969
- [21] Yates, J. *Fundamentals of Fluidized-Bed Chemical Processes*; Butterworths: London, 1983.
- [22] Werther, J, Mathematical Modelling of Fluidized Bed Reactor, Int. Chem. Eng, 20, 529-40, 1980
- [23] Werther, J., Hegner, B., Determination of Optimum Operating Conditions of Industrial Fluidized-bed Reactors, Int. Chem. Eng., 21, 585-598, 1981
- [24] Van Deemter, J., Mixing And Contacting In Gas-Solid Fluidized Beds Chem. Engng. 20, 529-541, 1961
- [25] Orcutt, J., C., Davidson, J., F., and Pigford, R., L., Reaction Time Distributions In Fluidized –Bed Catalytic Reactor .Chem. Engng Sci. 37, 553-565, 1962
- [26] Pereria, J., Chandrasekharan, K., and Calderbank, P., H., A Revised Model For Predicting The Performance Of A Fluidized Bed Reactor ,Chem., Engng. Sci., 37, 553-565, 1981
- [27] Swaaij, W., P., M., Van., 1985, Chemical Reactors In Fluidization (Edited By J.F. Davidson , R. Clift

- and D.Harrison),pp.595-629,1985,Academic Press New York
- [28] Dry,D.,J.,and Judd,M.,R.,Fluidized Beds Of Fine Dense Powders:Scale-up And Reactor Modelling .,Powder Technol.43, 41-53,1985
- [29] Horio,M.and Wen,C.,Y.,An Assessment of Fluidized Bed Modelling., A.I.C.h.E.,J.,Symp.,Ser.,73, 9-21,1977
- [30] Chavarie ,C.,and Grace ,J.R.,Performance Analysis of Fluidized Bed Reactor .,Ind.,Eng. Chem. Fundam. 14, 75-91,1975
- [31] Shaw ,I.,et al.,An Experimental Evaluation of Two- Phase Models Describing Catalytic Fluidized Bed Reactors.,A.,I.,C.,H.J.,Symp..Ser.70, 41-52,1974
- [32] Howmand, S.,and Davidson,J.F.,Chemical Conversion In A Slugging Fluidized Bed ,Trans.Instn. Chem. Engs.,46, T190-T203,1968