# MATHEMATICAL MODEL FOR FLUIDIZED-BED REACTOR

SHIGEKATSU MORI and IWAO MUCHI

*Department of Iron and Steel Engineering*

(Received October 29, 1965)

## Introduction

Various two-phase models have been proposed hitherto, and this model is considered as the most typical mathematical model for fluidized-bed reactor. However, two-phase model is not only a macroscopic one but also involves some parameters which cannot be determined easily from the operating conditions, and so this model is not necessarily an excellent one[1].

In this report, "particle-bubble model" basing on the motion of particles and bubbles in gaseous-fluidized bed has been proposed, and from this model a fractional coversion could be determined reasonably by use of the operating conditions.

Experimental results on the fractional conversions of the catalytic reaction in fluidized-bed reactors which has been reported by other investigators[2][3] were agreed satisfactorily with calculated results based on our model.

## 1. Bubble-Density Distribution Function

It is well known that bubbles grow in size as they rise in gaseous fluidized bed, and frequency of bubble decreases with increase in the distance from the bottom of bed.

To show bubble-frequency distribution in a bed, the bubble-density distribution function $q(y)$ is defined as Eq. (1).

$$\int_0^1 q(y)dy = 1 \qquad (1)$$

where $y \equiv z/L_f$: non-dimensional distance from the bottom of bed.

Letting the total bubble-frequency in a bed is $Q$, then the bubble frequency in a differential height of bed $dy$ can be written as $Qq(y)dy$, and the number of bubbles passing through the total cross-sectional area at $y$ per unit time can be written as follows:

$$P = \frac{Q}{L_f} q(y) u_B(y) \qquad (2)$$

## 2. Physical Model of Fluidized Bed

We consider that a fluibized-bed consists of bubbles, aggregated particles around bubbles and uniformly dispersed particles far from bubbles ($D$. group), and that there is no particle in bubbles.

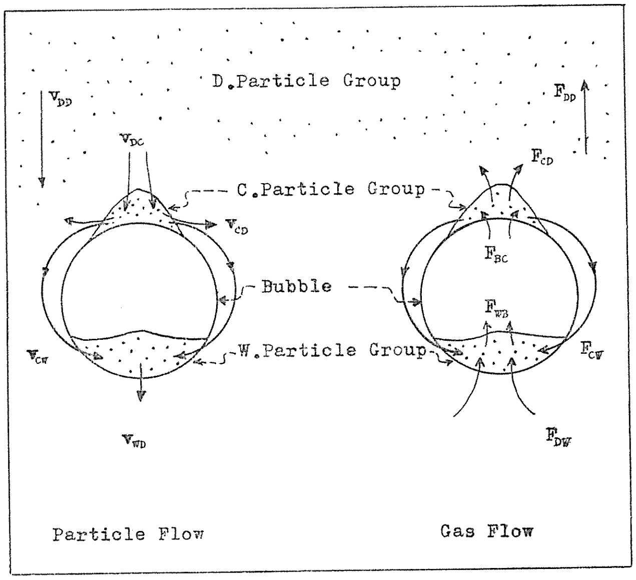


FIG. 1. Flow pattern of particle and gas.

One of the aggregated groups of particles (*C.* group) lies on the cap of a bubble and rises with it and the other one (*W.* group) lies under the bottom of the bubble and rises with it.

The flow patterns of gas and particles are illustrated in Fig. 1, where $F$ is the volume rate of flow of gas and $v$ is that of particles.

## 3. Derivation of Fundamental Equations

First-order irreversible reaction taking place under isothermal condition has been considered here.

Material balances around the differential height of a bed for each particle group and bubbles can be written as follows:

i) Balance on gas volume

(*C.* groups) $$\frac{\varepsilon_C}{L_f}\frac{d}{dy}(qu_B V_C) + q(F_{CD} + F_{CW} - F_{BC}) = 0 \tag{3}$$

(*W.* groups) $$\frac{\varepsilon_W}{L_f}\frac{d}{dy}(qu_B V_W) + q(F_{WB} - F_{CW} - F_{DW}) = 0 \tag{4}$$

(Bubbles) $$\frac{1}{L_f}\frac{d}{dy}(qu_B V_B) + q(F_{BC} - F_{WB}) = 0 \tag{5}$$

(*D.* group) $$\frac{d}{dy}F_{DD} + Qq(F_{DW} - F_{CD}) = 0 \tag{6}$$

ii) Balance on particle volume

(*C.* groups) $$\frac{(1-\varepsilon_C)}{L_f}\frac{d}{dy}(qu_B V_C) + q(v_{CW} + v_{CD} - v_{DC}) = 0 \tag{7}$$

(*W*. groups) $$\frac{(1-\varepsilon_W)}{L_f}\frac{d}{dy}(qu_B V_W)+q(v_{WD}-v_{CW})=0 \tag{8}$$

(*D*. group) $$\frac{d}{dy}v_{DD}+qQ(v_{DC}-v_{CD}-v_{WD})=0 \tag{9}$$

iii) Material balance on reactant

(*C*. groups) $$\frac{\varepsilon_C}{L_f}\frac{d}{dy}(qu_B V_C C_C)+q\{(F_{CD}+F_{CW})C_C-F_{BC}C_B\}+k(1-\varepsilon_C)\rho_p q V_C C_C=0 \tag{10}$$

(*W*. groups) $$\frac{\varepsilon_W}{L_f}\frac{d}{dy}(qu_B V_W C_W)+q(F_{WB}C_W-F_{CW}C_C-F_{DW}C_D)+k(1-\varepsilon_W)\rho_p q V_W C_W=0 \tag{11}$$

(Bubbles) $$\frac{1}{L_f}\frac{d}{dy}(qu_B V_B C_B)+q(F_{BC}C_B-F_{WB}C_W)=0 \tag{12}$$

(*D*. group) $$\frac{d}{dy}(F_{DD}C_D)+Qq(F_{DW}C_D-F_{CD}C_C)+k(1-\varepsilon_D)\rho_p\{A_t L_f-qQ(V_B+V_C+V_W)\}C_D=0 \tag{13}$$

iv) Initial condition

$$C_B=C_C=C_D=C_W=1 \qquad \text{at } y=0. \tag{14}$$

The longitudinal distribution of the concentration of reactant can be obtained from Eq. (3)-(14).

And then fractional conversion can be given as follows:

$$\eta=1-\left\{\frac{F_{DD}}{F_t}C_D+\frac{Qqu_B}{F_t L_f}(V_B C_B+\varepsilon_C V_C C_C+\varepsilon_W V_W C_W)\right\}_{y=1} \tag{15}$$

### 4. Simplification of Preceding Model

Taking into account of a practical usefulness, three assumptions (i)-(iii) have been applied to the preceding model, namely:

i) The volume rate of flow of gas $F_{BB}$ through rising bubbles would not be varied with axial distance in the bed[4], namely:

$$F_{BB}=\frac{Qq}{L_f}u_B V_B=\text{const} \tag{16}$$

ii) The volume ratio of *C*. group to a bubble $\delta_C$ and that of *W*. group to a bubble $\delta_W$ would be constant longitudinally[5], namely:

$$\delta_C=V_C/V_B=\text{const.}, \qquad \delta_W=V_W/V_B=\text{const.} \tag{17}$$

iii) The ratio of gas flow rate from *C*. group to *D*. group to that from a bubble to *C*. group would be constant in axial distance, namely:

$$\lambda=F_{CD}/F_{BC}=\text{const.} \tag{18}$$

Using these assumptions, the balance on the total volume rate of flow of gas at $y$ can be given as Eq. (19), and Eq. (20) can be derived from Eq. (3)-(7).

$$F_{DD} = F_t - F_{BB}(1 + \varepsilon_C\delta_C + \varepsilon_W\delta_W) \tag{19}$$

$$F_{WB} = \frac{F_{DW}}{\lambda} = \frac{F_{CD}}{\lambda} = \frac{F_{CW}}{1-\lambda} = F_{BC} \tag{20}$$

So Eq. (10)-(13) can be simplified as Eq. (21)-(24) by use of Eq. (16), (17), (18) and (20).

$$\frac{dC_B}{dy} = -F_{BCr}(C_B - C_W) \tag{21}$$

$$\frac{dC_C}{dy} = -\frac{F_{BCr}}{\varepsilon_C\delta_C}(C_C - C_B) - \frac{L_f k(1-\varepsilon_C)\rho_p}{\varepsilon_C u_B} C_C \tag{22}$$

$$\frac{dC_W}{dy} = -\frac{F_{BCr}}{\varepsilon_W\delta_W}\{C_W + C_D - (1-\lambda)C_C\} - \frac{L_f k(1-\varepsilon_W)\rho_p}{\varepsilon_W u_B} C_W \tag{23}$$

$$\frac{dC_D}{dy} = -\frac{\lambda F_{BB}}{F_{DD}} F_{BCr}(C_D - C_C) - \frac{L_f k(1-\varepsilon_D)\rho_p}{F_{DD}}\left\{A_t - F_{BB}(1+\delta_C+\delta_W)\frac{1}{u_B}\right\}C_D \tag{24}$$

Where $F_{BCr}$ is the ratio of the total volume rate of gas exchange between bubbles and its surrounding particles to the gas flow rate $F_{BB}$, and defined as Eq. (25)

$$F_{BCr} = \frac{QqF_{BC}}{F_{BB}} = \frac{L_f F_{BC}}{V_B u_B} \tag{25}$$

If $V_B$, $u_B$ and $F_{BC}$ are known as a function of $y$, Eq. (21)-(24) can be easily solved with initial condition Eq. (14).

Bubble diameter $D_B$ can be represented as the function of $y$, namely[6)7)8)]:

$$D_B = ay + b \tag{26}$$

Eq. (27)-(29) have been derived basing on the profile of bubbles and aggregated groups of particles illustrated as Fig. 2.

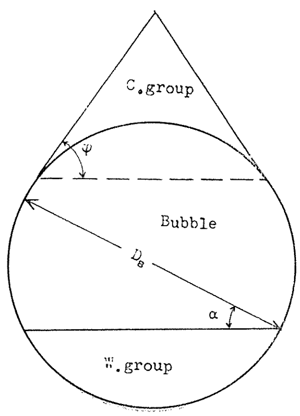


FIG. 2. Shape of bubble and groups of particle.

$$V_B = \frac{\pi}{12}(1+1.5 \sin\alpha - 0.5 \sin^3\alpha)\cdot D_B^3 \tag{27}$$

$$\delta_W = 1 - 2/(1+1.5 \sin\alpha - 0.5 \sin^3\alpha) \tag{28}$$

$$\delta_C = \frac{(\sin^2\varphi/\cos\varphi - 2 + 2\cos\varphi)}{(2+3\sin\alpha - \sin^3\alpha)} \tag{29}$$

Where the value of $\alpha$ is about 15–35° [5) 8)].
Rising velocity of bubble $u_B$ can be given as Eq. (30) [5) 8) 9) 10)].

$$u_B = u\sqrt{gD_B} \qquad u: \text{const.} \tag{30}$$

In order to represent the gas-exchange rate $F_{BC}$ between bubbles and its surrounding particles as the function of $y$, Eq. (31)-(33) have been assumed as follows:

i) Reaction between the flow rates of gas and particles from *C.* group to *W.* group would be given as Eq. (31).

$$F_{CW} = \frac{\varepsilon_C}{1-\varepsilon_C} v_{CW} \tag{31}$$

ii) The ratio of volume rate of flow of particles from *C.* group to *W.* group to that from *C.* group to *D.* group would be constant, namely:

$$\sigma = v_{CW}/v_{CD} = \text{const.} \tag{32}$$

iii) Volume rate of flow of particles from *D.* group to *C.* group would be given as follows:

$$v_{DC}(y) = A_{DC}(y) u_B (1-\varepsilon_D) \tag{33}$$

where $A_{DC}$ can be estimated as Eq. (34) [11)]

$$A_D\,(y) = 0.39 D_B^2 \left\{ \log\left( \frac{\rho_p d_p^2}{18\,\mu_f} \cdot \frac{u_B}{D_B} \right) + 1.24 \right\} \tag{34}$$

Using Eq. (31)-(33), the balance of total volume rate of flow of particles at $y$ can be written as Eq. (35), and then Eq. (36) can be derived from Eq. (7)-(9).

$$v_{DD} = F_{BB}\{\delta_C(1-\varepsilon_C) + \delta_W(1-\varepsilon_W)\} \tag{35}$$

$$v_{CW} = \frac{\sigma}{1+\sigma} v_{DC} \tag{36}$$

Finally $F_{BC}$ has been represented by use of Eq. (20), (31), (33) and (36), as follows:

$$F_{BC} = \frac{1-\varepsilon_D}{1-\lambda} \cdot \frac{\sigma}{1+\sigma} \cdot \frac{\varepsilon_C}{1-\varepsilon_C} u_B A_{DC} \tag{37}$$

Thus we can get the solution of Eq. (21)-(24).
Now, using the relations of Eq. (1), (16) and (26), the bubble-density distribution function $q(y)$ can be given as follows:

$$q(y) = \gamma D_B^{-7/2} = \gamma(ay+b)^{-7/2} \tag{38}$$

where
$$\gamma = \frac{5}{2} ab^{5/2} \frac{1}{\left\{1-\left(\frac{b}{a+b}\right)^{5/2}\right\}} \tag{39}$$

## 5. Comparison with Experimental Results

Using the experimental data and a parameter $\lambda$ determined from the data of the conversions observed, it is possible to evaluated the fractional conversion of

TABLE 1. Calculated results

| Data | $u_0/u_{mf}$ | $F_{er}$ | $X$ | $\eta_{exp}$ | $\lambda_{exp}$ | $F_{BCr}$ |
|---|---|---|---|---|---|---|
| Shen[2] (1) | 2.58 | 0.35 | 0.34 | 0.26 | 0.73 | 0.90 |
| (2) | 4.28 | 0.19 | 0.20 | 0.17 | 0.82 | 0.90 |
| (3) | 4.99 | 0.15 | 0.18 | 0.14 | 0.81 | 0.80 |
| Massimilla[3] (1) | 2.40 | 0.39 | 0.46 | 0.30 | 0.74 | — |
| (2) | 3.20 | 0.27 | 0.35 | 0.26 | 0.86 | 0.72 |
| (3) | 4.80 | 0.16 | 0.24 | 0.18 | 0.86 | 0.55 |

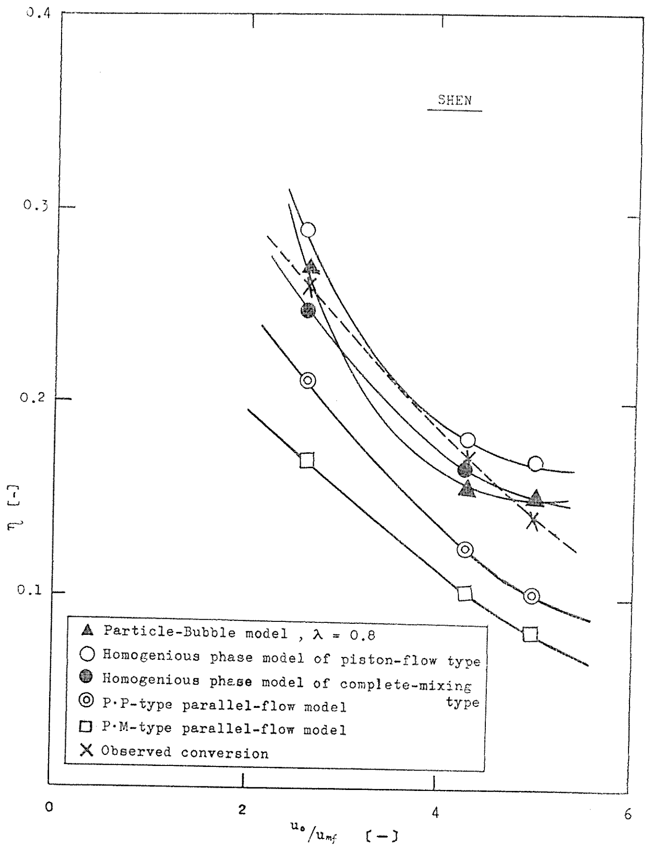


FIG. 3. Comparison of conversions calculated and those observed.

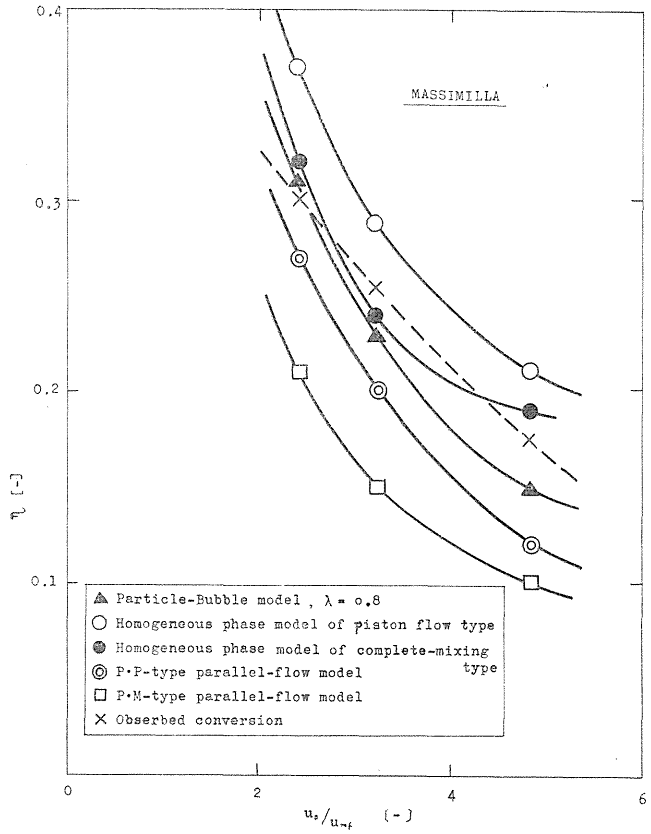


FIG. 4. Comparison of conversions calculated and those observed.

fluidized-bed reactor.

The data used in the calculation and the results obtained are given in Table 1. Where $\eta_{exp.}$ is the conversion observed, $X = kW_s/F_t$, $F_{er} = 1 - F_{BB}/F_t$[8], and the value of $\lambda_{exp.}$ calculated from $\eta_{exp.}$ are given as about 0.8.
$F_{Br}$ is the ratio of the total volume rate of exchange of gas between bubbles and those surrounding particles in the bed to the total gas rate of flow $F_t$, namely:

$$F_{Br} = \frac{1}{F_t}\int_0^1 QqF_{BC}dy = \frac{F_{BB}}{F_t}\int_0^1 F_{BCr}dy \qquad (40)$$

These calculated results are compared with other models[8] in Fig. 3 and 4.
Taking $\lambda = 0.8$ for our model, the calculated results of fractional conversions are good agreed with the observed data.

Fig. 5 shows the relation between parameter $\lambda$ and conversion $\eta$: $\eta_{exp.}$ and $\lambda_{exp.}$ given by Shen[2] ($u_0/u_{mf} = 2\ 58$) are 0.26 and 0.73, respectively.

And the effect of $\lambda$ on $\eta$ increases with increase in $\lambda$, but this effect is slight in the range of small $\lambda$.

Both the relations between bubble-density function $q$ and $y$, and between $D_B$ and $y$ are shown in Fig. 6.

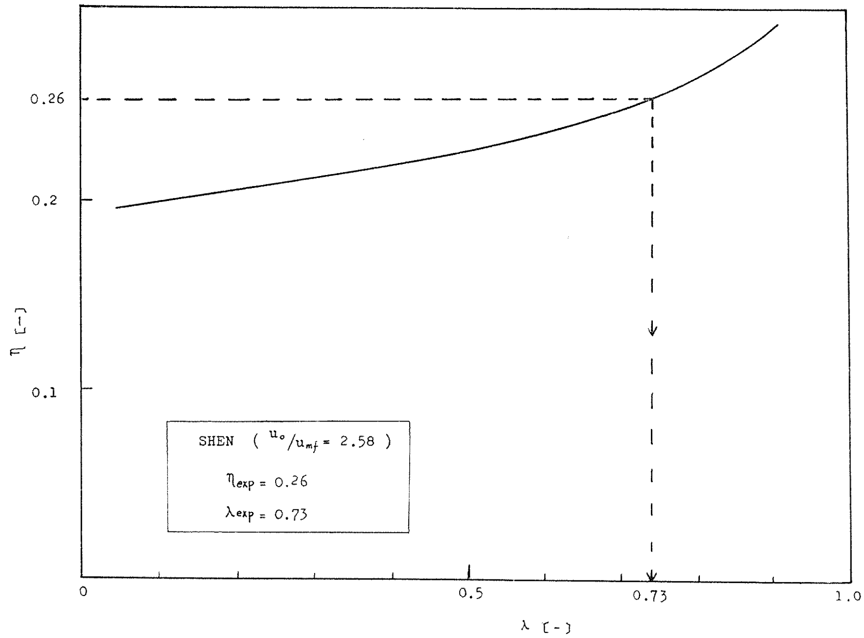


FIG. 5. $\eta$ vs. $\lambda$

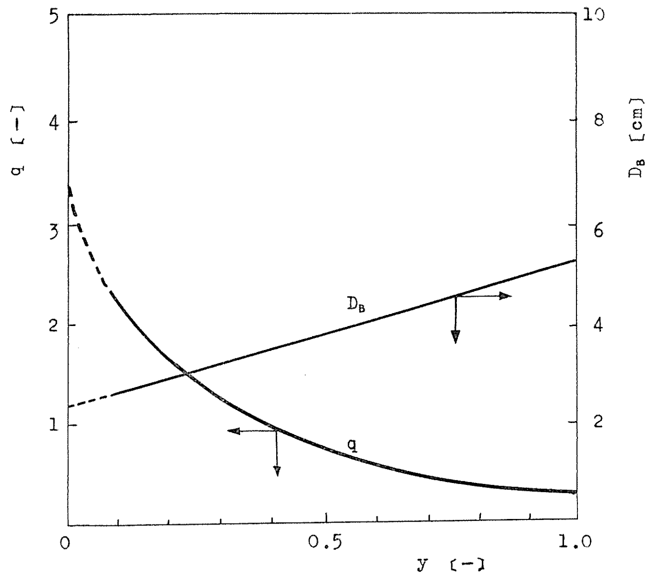


FIG. 6. $q$ vs. $y$ and $D_B$ vs. $y$

From Fig. 6 it can be found that $q$ is large at bottom and decreases extremely as distance from the bottom increases, and gas-exchange ratio $F_{BCr}$ is large at bottom and small at top.

Also the concentration distribution of reactant in each particle group in

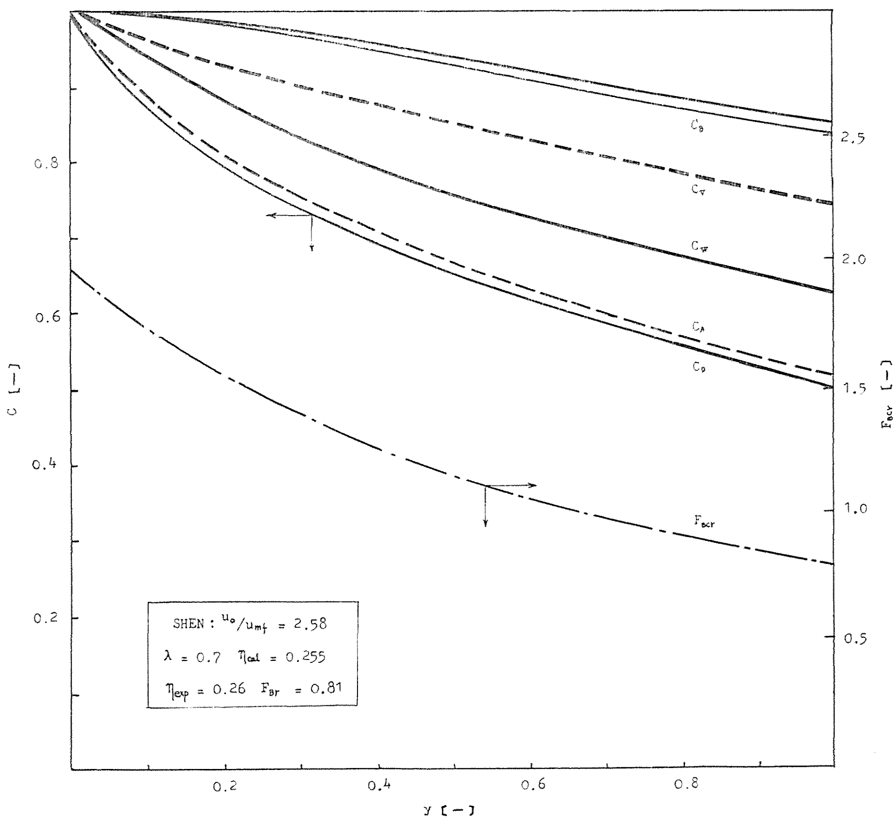


FIG. 7. Concentration distributions and $F_{BCr}$ vs. $y$.

the reactor is illustrated in Fig. 7, and where $C_A$ and $C_V$ are mean concentration at $y$ given as Eq. (41) and (42), respectively.

$$C_A = \frac{(F_{BB}/u_B)(C_B + \varepsilon_C\delta_C C_C + \varepsilon_W\delta_W C_W) + \varepsilon_D\{A_t - (F_{BB}/u_B)(1+\delta_C+\delta_W)\}C_D}{A_t\varepsilon_D + (F_{BB}/u_B)\{(1-\varepsilon_D)+(\varepsilon_C-\varepsilon_D)\delta_C+(\varepsilon_W-\varepsilon_D)\delta_W\}} \quad (41)$$

$$C_V = \frac{1}{F_t}\{F_{DD}C_D + F_{BB}(C_B + \varepsilon_C\delta_C C_C + \varepsilon_W\delta_W C_W)\} \quad (42)$$

Now, Eq. (15) can be written as follows:

$$\eta = 1 - C_{V(y=1)} \quad (43)$$

## Conclusion

"Particle-bubble model" basing on the behaviors of particles and bubbles has been proposed here as a mathematical model for fluidized-bed catalytic reactor.

It is guessed that this model is actually available for predicting the fractional conversion from the data of the operatig conditions.

## Notation

| | |
|---|---|
| $A_t$ | : total cross-sectional area of reactor [cm²] |
| $a$, $b$ | : constant defined by Eq. (26) [cm] |
| $C$ | : fractional concentration of reactant [−] |
| $D_B$ | : bubble diameter [cm] |
| $d_p$ | : particle diameter [cm] |
| $F$ | : volume rate of flow of gas [cm³/sec] |
| $F_{Br}$ | : dimensionless factor defined by Eq. (40) [−] |
| $F_{BCr}$ | $=QqF_{BC}/F_{BB}$ [−] |
| $F_t$ | : volume rate of flow of total gas in fluidized-bed reactor [cm³/sec] |
| $g$ | : gravitational acceleration [cm/sec²] |
| $k$ | : 1 st-order reaction rate constant [cm³/g(cat)·sec] |
| $L_f$ | : fluidized-bed height [cm] |
| $p$ | : number of bubbles passing through the total cross-sectional area at $y$ per unit time [1/sec] |
| $Q$ | : total bubble frequency in fluidized bed [−] |
| $q$ | : bubble-density distribution function [−] |
| $u_B$ | : rising velocity of bubble [cm/sec] |
| $u_{mf}$ | : superficial minimum fluidization velocity [cm/sec] |
| $u_0$ | : superficial gas velocity of fluidized bed [cm/sec] |
| $V$ | : volume [cm³] |
| $v$ | : volume rate of flow of particles [cm³/sec] |
| $W_s$ | : total mass of catalyst in fluidized-bed reactor [g] |
| $X$ | $=kW_s/F_t$ [−] |
| $y$ | $=z/L_f$ [−] |
| $z$ | : longitudinal distance from bottom of bed [cm] |
| $\alpha$ | : wake angle [deg] |
| $\delta$ | : ratio of volume [−] |
| $\varepsilon$ | : fractional void in group of particles [−] |
| $\eta$ | : fractional conversion [−] |
| $\lambda$ | $=F_{CD}/F_{BC}$ [−] |
| $\mu_f$ | : viscocity of gas [g/cm·sec] |
| $\rho_p$ | : dencity of particle [g/cm³] |
| $\sigma$ | $=v_{CW}/v_{CD}$ [−] |
| $\varphi$ | : angle of *C*. group of particles [deg] |

**Suffix**

| | |
|---|---|
| $B$ | : bubble |
| $C$ | : *C*. group (Cap) |
| $D$ | : *D*. group (Dispersed) |
| $W$ | : *W*. group (Wake) |

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