

SIMULATION OF AN INDUSTRIAL FLUIDIZED BED REACTOR USING A BUBBLE GROWTH MODEL

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In this paper we develop a model for simulation and design of large scale industrial fluidized bed reactors. The suggested procedure is based on the following key concepts and assumptions: (i) bubbles formed at the distributor grow with height and this variation can be described by the physical picture due to Darton et al.¹, (ii) the bubble growth is limited to a maximum, equilibrium, bubble size depending mainly on the particle and particle size distribution, (iii) the rise velocity of a bubble of any given size is dependent on the scale of operation, i.e. vessel diameter, and (iv) the interphase mass transfer between a bubble and the surrounding dense phase is the result of two contributions: throughflow and diffusion, which are modelled following the approach of Davidson et al.².

It is suggested in the procedure that the key model parameters such as the equilibrium bubble size and dense phase gas velocity be determined in "cold flow" simulation experiments carried out in columns of reasonably large size, say larger than 0.6 m diameter.

The developed model is used to simulate the performance of an industrial fluidized bed reactor for the oxidation of HCl to produce Cl₂. The gas phase conversion (as measured in an industrial unit of diameter 2.9 m and expanded bed height of 10 m, operating at a superficial gas velocity of 0.2 m s⁻¹) has been reported to be strongly dependent on the % of "fines", i.e. particles smaller than 44 μm. Since the presence of such "fine" particles is known to have bubble breaking tendencies, the simulations of the fluid bed unit was carried out by allowing the equilibrium bubble size to vary. The model parameters chosen in the simulations were based on experimentally available information on cold flow simulation experiments. The model calculations show that the observed influence of % fines (conversion falling from 95.7% to only 91% with decrease in fines content from 20% to 7%) can be rationalized by allowing the equilibrium size to decrease with increasing fines content. The equilibrium bubble sizes thus determined depend on the initial bubble size formed at the distributor and varies from 0.11–0.17 m; this variation is within the range of equilibrium bubble sizes measured by several workers and therefore provides verification, if indirect, of the model approach.

INTRODUCTION

Fluidized bed reactor modelling has been the subject of numerous papers and books; see for example the recent works of Davidson, Clift and Harrison³ and Geldart⁴. There is general agreement that the models have to take proper account of bubble hydrodynamics, especially the phenomena of bubble growth (Krishna⁵, van Swaaij⁶, Werther⁷).

Use of the bubble growth models requires information on several parameters characterizing the solids and the vessel; *a priori* estimation of these model parameters is not possible in general and it is generally agreed that these will need to be measured in "cold flow" experimental units of a reasonably large size say greater than 0.6 m in diameter (Krishna⁵).

In this paper we develop a simulation model for an industrial fluidized bed reactor carrying out a first order irreversible reaction. The model is used to simulate the behaviour of an industrial fluid bed reactor for the oxidation of HCl to produce Cl₂, the data for which has been published by De Vries et al.⁸. The simulation of the performance of this industrial reactor (of diameter 2.9 m and expanded height 10 m) should prove to be a good test of the physical model chosen for the reactor in view of the very strong influence observed for the influence of "fines", i.e. catalysts smaller than 44 μm, on the conversion levels achieved; see Figure 1. Thus, *under nearly identical operating conditions*, the gas phase conversion falls from 95.7% to only 91% when the % "fines" in the

vessel decreases from 20% to 7%. Even without a deeper analysis, it should be apparent that the chosen model for simulating the performance of this unit will only be successful if it is capable of explaining the influence of particle size and size distribution on the bubble hydrodynamics. Now, it is well recognized that the particle size and size distribution affects significantly the maximum, or equilibrium, bubble size obtained in a fluid bed (Clift⁹) and so it becomes apparent that the correct modelling approach would be to make proper allowance for the growth of bubbles above the distributor, limited to the maximum, stable, bubble size.

MODEL DEVELOPMENT

We choose the two-phase model for describing the fluid bed reactor, following in essence the approach of May¹⁰ and van Deemter¹¹. The two "phases" are identified as follows (see Figure 2):

—the "dilute" phase consisting of bubbles traversing up the column in plug flow, and exchanging gaseous species with

—the "dense" phase consisting of the solids (e.g. catalyst) kept in suspension by gas at a velocity U_{df} . The remainder of the gas, at a velocity $(U - U_{df})$ flows up through the "dilute" or bubble phase. The dense phase of solids and gas are assumed to be backmixed with an axial dispersion coefficient D_{ax} .

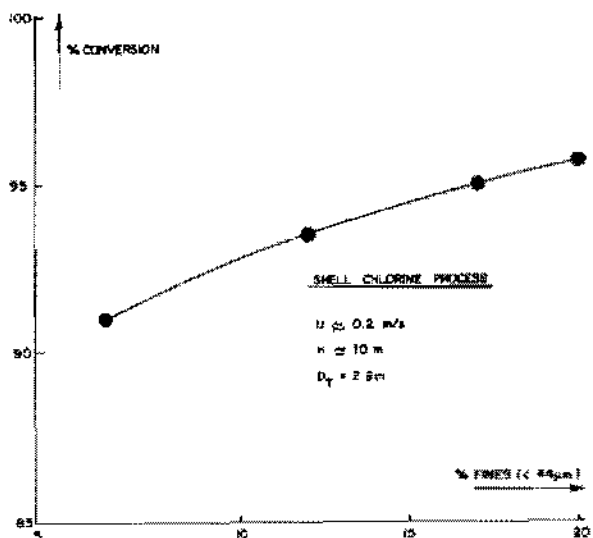


Figure 1. Conversion of HCl as a function of % fines, obtained in a commercial fluid bed reactor (De Vries et al⁸).

We now take up the question of providing a more detailed description of the above physical picture so as to allow the prediction of the gas phase conversion in a reactor of given dimensions, under specified operating conditions.

Estimation of Bubble Size and Bubble Rise Velocity

Bubbles formed at the distributor suffer coalescence as they rise up the column and therefore grow in size. There are many bubble growth models (see Clift⁹); we choose here the model due to Darton et al¹ which has a simple mechanistic base. According to the Darton model, the diameter of a sphere having the same volume as the actual bubble is given by the relation:

$$d_b = \alpha_1 (U - U_{df})^{2/5} (h + h_0)^{4/5} g^{-1/5} \tag{1}$$

where α_1 is a constant, found by data fitting to be 0.54; h is the height above the distributor and h_0 characterizes the distributor inasmuch as it determines the size of the bubble formed at the distributor plate ($h = 0$):

$$d_{b0} = \alpha_1 (U - U_{df})^{2/5} h_0^{4/5} g^{-1/5} \tag{2}$$

For porous plate distributors Darton¹ calculates $h_0 = 0.03 \text{ m}$ and for operation at $U = 0.2 \text{ m s}^{-1}$ the value of $d_{b0} = 0.01 \text{ m}$. Industrial distributors would give initial bubble sizes larger than 0.01 m say between $0.02 - 0.1 \text{ m}$; see Clift⁹.

The bubble growth does not take place indefinitely and there is sufficient evidence in the literature to suggest that, depending on the particle and particle size distribution, there exists a stable, equilibrium, size for the bubble, d_b^* . We shall denote the value of h for which $d_b = d_b^*$ as h^* , i.e.

$$d_b^* = \alpha_1 (U - U_{df})^{2/5} (h^* + h_0)^{4/5} g^{-1/5} \tag{3}$$

For values of h greater than h^* , the bubble size stays constant at the value d_b^* , given by equation (3); see Figure 3.

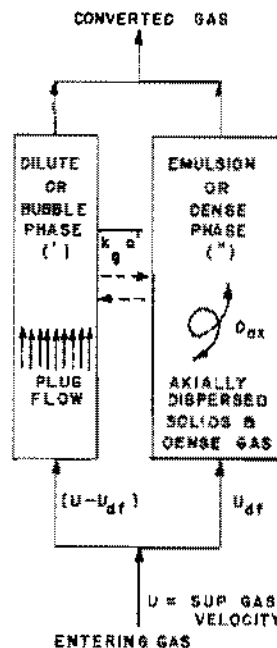


Figure 2. Two-Phase model for fluidized bed after May¹⁰ and van Deemter¹¹.

Werther⁷ carried out extensive measurements in fluid beds of different diameters and found that the rise velocity of a bubble of a given size was dependent on the size of the vessel D_T . The large scale eddies present in a large diameter bed (the size of the largest eddy is roughly equal to the diameter of the vessel) tend to accelerate the bubble rise. In smaller sized columns this effect is present only to a limited extent. On the basis of his experimental data, obtained in beds ranging from 0.1 to 1 m in diameter, Werther⁷ proposed the following correlation for the bubble rise velocity:

$$V_b = \phi \sqrt{g d_b} \tag{4}$$

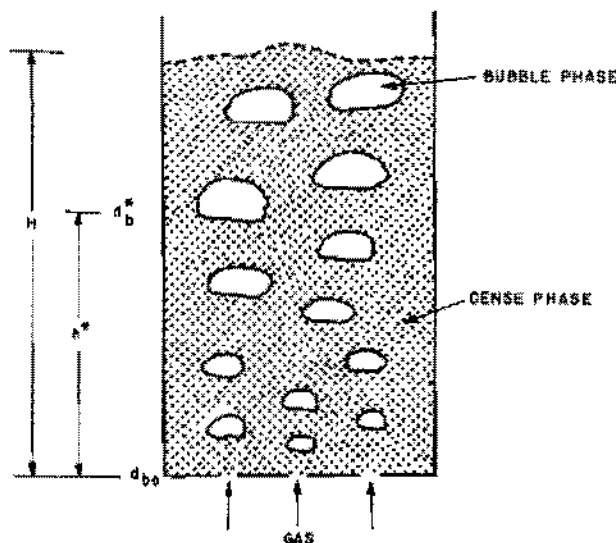


Figure 3. Bubble growth model for fluid bed wherein the growth is restricted to a diameter d_b^* .

where the constant ϕ is dependent on the column diameter as follows:

$$\phi = \phi_1 \quad \text{for } D_T \leq 0.1 \text{ m} \quad (5a)$$

$$\phi = \phi_2 D_T^{0.4} \quad \text{for } 0.1 \leq D_T \leq 1 \text{ m} \quad (5b)$$

$$\phi = \phi_2 \quad \text{for } D_T > 1 \text{ m} \quad (5c)$$

where the constants ϕ_1 and ϕ_2 are:

$$\phi_1 = 1; \phi_2 = 2.5 \text{ for Geldart type } A \text{ powders}$$

$$\phi_1 = 0.64; \phi_2 = 1.6 \text{ for Geldart type } B \text{ powders} \quad (6)$$

Careful measurements of the bubble rise velocity by Roes and Garnier¹² have provided independent support of the use of the combination of equations (1)–(5) for estimation of V_b and also the superiority of the Werther correlation over the more commonly used expression (see for example Davidson et al²):

$$V_b = U - U_{dr} + 0.711 \sqrt{g d_b} \quad (7)$$

Hold-up of "dilute" and "dense" Phases

The dilute or bubble phase hold-up, $\bar{\epsilon}_b$, averaged over the fluid bed height h is

$$\bar{\epsilon}_b = \frac{1}{H} \int_0^H \frac{(U - U_{dr})}{V_b} dh \quad (8)$$

Equations (1) and (4) may be substituted in equation (8) to obtain the bubble hold-up; the integration must be performed in two parts: $0 - h^*$ and $h^* - H$, with the restriction that in the latter region d_b^* remains constant. The results are given below:

$$\bar{\epsilon}_b = \alpha_2 [(H + h_0)^{3/5} - h_0^{3/5}] \quad \text{for } H \leq h^* \quad (9a)$$

and

$$\begin{aligned} \bar{\epsilon}_b = \alpha_2 [(h^* + h_0)^{3/5} - h_0^{3/5}] / (3/5) \\ + \alpha_2 [(h^* + h_0)^{-2/5}] [H - h^*] \quad \text{for } H > h^* \end{aligned} \quad (9b)$$

where

$$\alpha_2 = \phi^{-1} \alpha_1^{-1/2} (U - U_{dr})^{4/5} H^{-1} g^{-2/5} \quad (9c)$$

The important parameter d_b^* , or equivalently the equilibration height h^* , must be determined experimentally for any given powder. The procedure for the determination of this parameter is discussed by Krishna⁵ and Roes and Garnier¹² and consists of performing dynamic gas disengagement experiments in a fairly large scale diameter (preferably larger than 0.6 m) "cold flow" simulation column. This type of experiments allows direct determination of $\bar{\epsilon}_b$, the dense phase expansion, ϵ_{dr} and the dense phase gas velocity U_{dr} . Fitting of a series of $\bar{\epsilon}_b - H$ data allows determination of h^* , or equivalently d_b^* . It is to be noted here that there are no reliable models for prediction of ϵ_{dr} and U_{dr} and these have to be determined experimentally by dynamic gas disengagement experiments. The parameter U_{dr} is a particularly important one for estimation of the interphase mass transfer rates, as we shall see.

Roes and Garnier¹² were able to correlate their $\bar{\epsilon}_b$ data successfully by use of equation (9), providing partial support for the approach suggested here.

Interphase Mass Transfer

The gaseous mass exchange between the bubble phase and the dense phase is the result of two, additive, mechanisms of throughflow and diffusion (see Grace¹³ and Davidson et al²). The volumetric mass transfer coefficient $k_g a'$, defined per unit volume of the bubble phase, is given by:

$$k_g a' = \alpha_3 U_{dr} d_b^{-1} + \alpha_4 d_b^{-5/4} \quad (10a)$$

where

$$\alpha_3 = 7.14; \quad \alpha_4 = 5.46 D_G^{1/2} g^{1/4} \left[\frac{\epsilon_{dr}''}{1 + \epsilon_{dr}''} \right] \quad (10b)$$

In the reactor model the dimensionless group which quantifies the mass transfer effect is the number of mass transfer units, NTU , defined as

$$NTU = v \frac{k_g a' H}{V_b} \quad (11)$$

where v is the fraction of the total gas flow which traverses up the column in the form of bubbles:

$$v = (U - U_{dr})/U \quad (12)$$

Since both $k_g a'$ and V_b vary up the height of the bed, the integral average NTU may be calculated from

$$\overline{NTU} = v \int_0^H \frac{k_g a'}{V_b} dh \quad (13)$$

Incorporating the relations (1), (4), (5) and (11) in equation (13), the integrations may be carried out for the two cases $H \leq h^*$ and $H > h^*$ to yield:

$$\begin{aligned} \overline{NTU} = \alpha_5 [h_0^{-1/5} - (H + h_0)^{-1/5}] \\ + \alpha_6 [h_0^{-2/5} - (H + h_0)^{-2/5}] \quad \text{for } H \leq h^* \end{aligned} \quad (14a)$$

and

$$\begin{aligned} \overline{NTU} = 5\alpha_5 [h_0^{-1/5} - (h^* + h_0)^{-1/5}] \\ + \frac{5}{2}\alpha_6 [h_0^{-2/5} - (h^* + h_0)^{-2/5}] + [\alpha_5 (h^* + h_0)^{-6/5} \\ + \alpha_6 (h^* + h_0)^{-7/5}] [H - h^*] \quad \text{for } H > h^* \end{aligned} \quad (14b)$$

where

$$\alpha_5 = v \alpha_3 \phi^{-1} g^{-1/5} \alpha_1^{-3/2} (U - U_{dr})^{-3/5} U_{dr} \quad (14c)$$

and

$$\alpha_6 = v \alpha_4 \phi^{-1} g^{-3/20} \alpha_1^{-7/4} (U - U_{dr})^{-7/10} \quad (14d)$$

For the determination of \overline{NTU} using equation (14) the parameter inputs required are h^* (or equivalently d_b^*), h_0 (or equivalently d_{b0}), U_{dr} and the void fraction of the dense phase ϵ_{dr}'' .

Dense Phase Backmixing

While the fast rising bubbles traverse the column in plug flow, the dense phase which derives energy from the rising bubbles gets "churned" up. The size of the eddies which causes this churning or mixing process is limited in size by the diameter of the vessel. Thus larger diameter

vessels experience a much greater mixing effect. From a scale-up point of view this mixing effect is vital as it has an impact on the conversion achieved in a fluid bed of a given height. The dimensionless group characterising the extent of mixing or staging in the dense phase is NMU , the number of mixing units:

$$NMU = \frac{UH}{fD_{ax}} \quad (15)$$

where D_{ax} is the axial dispersion coefficient, a reasonable estimate of which, for design and scale-up purposes, can be obtained from the Baird and Rice¹⁸ correlation:

$$D_{ax} = 0.35(gU)^{1/3} D_T^{2/3} \quad (16)$$

The factor f in equation (15) represents the fraction of the total reactor volume occupied by the dense phase gas; this can be calculated from the bubble hold-up, $\bar{\epsilon}_b$, (cf. equations (8), (9)) and the dense phase expansion ϵ_{df} :

$$f = (1 + \epsilon_{df} - \rho_b/\rho_p)/(1 + \epsilon) \quad (17)$$

where the total bed expansion ϵ is given by

$$\epsilon = (\epsilon_b + \epsilon_{df})/(1 - \epsilon_s) \quad (18)$$

Figure 4 shows some typical calculations of NMU as a function of the reactor diameter D_T . For NMU values less than about 1, the dense phase may be considered to be completely well mixed; this situation is typical of large diameter industrial fluid beds with H/D_T of less than about 2. Small diameter (e.g. pilot plant) reactors having fluid bed heights of 2–3 m may have NMU values exceeding about 5 and the dense phase may be considered to be in plug flow, with consequent beneficial effect on the reactor conversion. This is a vital aspect to be reckoned with in scale-up from pilot to commercial scale operation.

Number of Reaction Units

For a first order irreversible reaction, the dimensionless group which describes the reaction rate is NRU , the number of reaction units:

$$NRU = \frac{k_{pb}H}{(1 + \epsilon)U} \quad (19)$$

which k_{pb} is the first order rate constant as would be determined in a packed bed microflow reactor and defined in terms of the volume of a packed bed of particles.

Mathematical Model

The differential equations describing the variation of the model fractions of component A , which undergoes irreversible first-order reaction on the solid particle, for the dilute and dense phases are:

$$\frac{dx'}{d\xi} + \frac{1}{v} NTU(x' - x'') = 0 \quad (20)$$

and

$$\frac{d^2x''}{d\xi^2} - NMU(1 - v) \frac{dx''}{d\xi} - NMU(NTU + NRU)x'' + NMUNTUx' = 0 \quad (21)$$

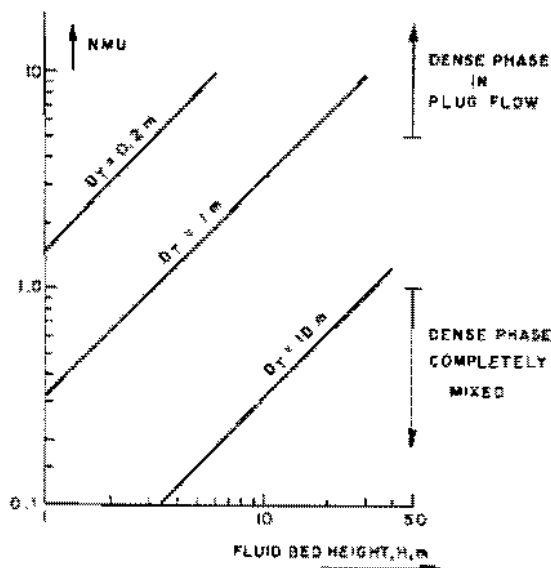


Figure 4. Number of mixing units NMU as a function of fluid bed height and diameter.

with the boundary conditions:

Inlet ($\xi = 0$)

$$\begin{aligned} x' \Big|_{\xi=0^+} &= x' \Big|_{\xi=0^-} \\ &= x_{in} \text{ (entering gas composition)} \end{aligned} \quad (22a)$$

$$\begin{aligned} x'' \Big|_{\xi=0^-} &= x'' \Big|_{\xi=0^+} \\ - \left[\frac{1}{1-v} \right] \left[\frac{1}{NMU} \right] \frac{dx''}{d\xi} \Big|_{\xi=0^+} &= x_{in} \end{aligned} \quad (22b)$$

Outlet ($\xi = 1$)

$$\begin{aligned} \frac{dx'}{d\xi} \Big|_{\xi=1} &= 0; \quad \frac{dx''}{d\xi} \Big|_{\xi=1} = 0; \\ x_{out} &= vx' \Big|_{\xi=1} + (1-v)x'' \Big|_{\xi=1} \end{aligned} \quad (22c)$$

The conversion of A is then

$$\chi = 1 - x_{out}/x_{in} \quad (23)$$

The conversion of species A undergoing the first order irreversible reaction is seen from equations (20)–(23) to be a function of four dimensionless groups: v , NTU , NMU and NRU . The number of transfer units NTU , in particular, varies along the height of the column. If the integral averaged value \overline{NTU} , cf. equation (14), then the set of equations (20)–(23) may be solved analytically¹⁵. We present below the solutions in two cases of practical interest: (i) the general case in which the dense phase is axially dispersed with a dispersion coefficient D_{ax} and (ii) the case in which the dense phase is completely mixed, of interest for large scale industrial reactors.

(i) *Axially dispersed dense phase*

$$\chi = 1 - \sum_{i=1}^3 \frac{N_i}{|Q|} \left[v \left(\frac{a_i}{\lambda_i + a_i} \right) + (1-v) \right] \exp(\lambda_i) \quad (24)$$

where the following parameters have been defined:

$$\begin{aligned} a_1 &= \overline{NTU}/v; & a_2 &= a_1; & b_1 &= -(1-v)NMU; \\ b_2 &= -NMU(\overline{NTU} + NRU) \\ b_3 &= -NMU\overline{NTU} \end{aligned} \quad (25)$$

λ_j are the roots of the cubic equation:

$$\lambda^3 + (a_1 + b_1)\lambda^2 + (a_1b_1 + b_2)\lambda + (a_1b_2 - a_2b_3) = 0 \quad (26)$$

The matrix $[Q]$ has the elements:

$$\begin{aligned} q_{1j} &= a_2/(\lambda_j + a_1); & q_{2j} &= (\lambda_j + b_1)/b_1; \\ q_{3j} &= \lambda_j \exp(\lambda_j), & j &= 1, 2, 3 \end{aligned} \quad (27)$$

and the elements N_i are given by

$$N_1 = \begin{vmatrix} q_{22} & q_{23} \\ q_{32} & q_{33} \end{vmatrix} - \begin{vmatrix} q_{12} & q_{13} \\ q_{32} & q_{33} \end{vmatrix} \quad (28a)$$

$$N_2 = \begin{vmatrix} q_{21} & q_{22} \\ q_{31} & q_{32} \end{vmatrix} - \begin{vmatrix} q_{11} & q_{12} \\ q_{31} & q_{32} \end{vmatrix} \quad (28b)$$

$$N_3 = \begin{vmatrix} q_{21} & q_{22} \\ q_{31} & q_{32} \end{vmatrix} - \begin{vmatrix} q_{11} & q_{12} \\ q_{31} & q_{32} \end{vmatrix} \quad (28c)$$

(ii) *Completely backmixed dense phase*

Here the composition of the dense phase x'' is uniform everywhere inside the reactor and given by the overall material balance as

$$\frac{x''}{x_m} = \chi/NRU \quad (29)$$

and the conversion is given by

$$\chi = \frac{(1 - v \exp(-a_1))NRU}{1 + NRU - v \exp(-a_1)} \quad (30)$$

where a_1 is defined by equation (25).

RESULTS OF SIMULATION OF THE SHELL CHLORINE PROCESS FLUID BED REACTOR

De Vries et al⁸ give results of the conversion of HCl obtained on oxidation by air to produce Cl₂ in a fluid bed reactor using silica catalyst (Shell Chlorine Process); see Figure 1. Data on the fluidization characteristics of the silica catalyst were also determined in "cold flow" model experiments in beds of diameters 0.6 and 1.5 m (see De Groot¹⁶ and De Vries et al⁸). From the data available in these papers the following fluidization parameters, properties and rate constants were taken in the calculations:

$$\begin{aligned} \epsilon_{df} &= 0.2; & c_{df}^0 &= 0.5; & \rho_b &= 600 \text{ kg m}^{-3}; \\ \rho_p &= 1200 \text{ kg m}^{-3}; & U_{df} &= 0.01 \text{ m s}^{-1}; \\ D_G &= 35 \text{ mm}^2 \text{ s}^{-1}; & k_{pb} &= 0.6 \text{ s}^{-1}. \end{aligned}$$

Two important parameters d_m^* and d_{b0} are still unknown. For a porous plate distributor, used in laboratories, the value of d_{b0} for operation at $U = 0.2 \text{ m s}^{-1}$ works out to 0.01 m following equation (2). Industrial distributors can be expected to produce initial bubble sizes larger than 0.01 m. As sufficient data on the

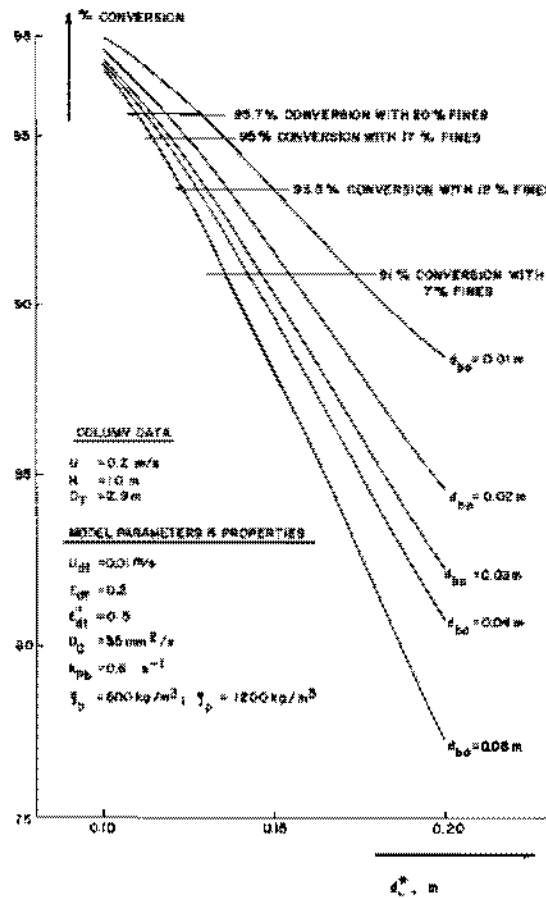


Figure 5. Results of simulations of reactor conversion as a function of the equilibrium bubble size d_b^* .

particular distributor used in the Shell Chlorine Process are not available, the simulations were performed for a range of d_{b0} values 0.01 – 0.08 m, which should cover the expected range for industrial units⁹. For any chosen value of d_{b0} the equilibrium stable bubble size was varied over the range of values and the conversion obtained was calculated using the analytic solution given by equation (24); the calculations are presented in Figure 5. The strong dependence of the conversion level on d_b^* and d_{b0} values is emphasized by the results of Figure 5.

From the observed dependence of the % conversion on the % fines (cf. Figure 1), we may relate d_b^* to the % fines, for any chosen value of d_{b0} ; this leads to the results shown in Figure 6. The interpretation of Figure 6 is as follows: if the dependence of d_b^* on % fines, for any d_{b0} value, is as shown in Figure 6, then the influence of % fines on the degree of conversion as depicted in Figure 1 can be rationalized. The simulation model presented in this paper is considered to be a realistic one because of the following two reasons:

(i) Figure 6 shows that increase in % fines decreases d_b^* . This trend is in line with the known physical effect of fines addition which tends to reduce the stability of bubbles leading to a smaller equilibrium bubble size⁹.

(ii) The range of d_b^* values obtained in Figure 6, 0.11–0.17 m is within the range of equilibrium bubble sizes to be expected for fine particles of average particle

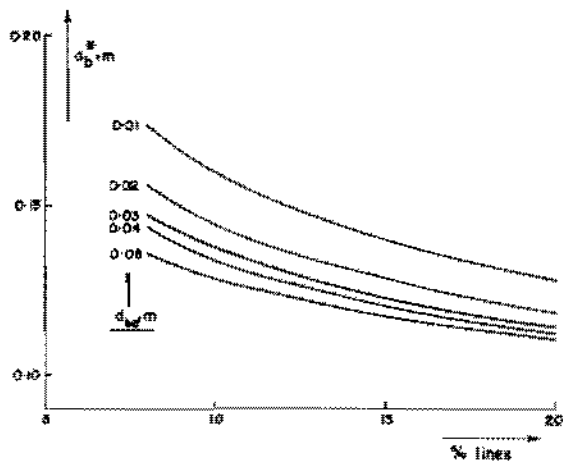


Figure 6. Equilibrium bubble size as a function of % fines obtained on comparison of simulation results of Figure 5 with plant data of Figure 1.

size of about $80 \mu\text{m}$ (see Cliff⁹). This provides indirect confirmation of the model developed in this paper.

For *a priori* prediction of the behaviour of large industrial reactors it is clearly necessary to have good estimates of both d_b^* and d_{b0} . By performing a series of dynamic gas disengagement experiments with the actual distributor to be used, it is possible to fit the $\bar{c}_b - H$ data to determine both d_b^* and d_{b0} ; the procedure is along the lines suggested by Roes and Garnier¹².

The model developed in this paper can also be used to demonstrate the enormous influence of the column diameter on the achievable conversion in a fluidized bed reactor. To demonstrate the influence of the scale of operation, calculations were performed for two units, both carrying out the oxidation of HCl to produce Cl_2 :

(i) a pilot plant scale reactor of diameter $D_T = 0.2 \text{ m}$ fitted with a porous plate distributor giving $d_{b0} = 0.01 \text{ m}$, and

(ii) a commercial scale unit of diameter $D_T = 2.9 \text{ m}$ (corresponding to the Shell Chlorine Process⁸), with a gas distributor device yielding $d_{b0} = 0.04 \text{ m}$.

In both reactors the equilibrium bubble size (dependent on the particle size and size distribution, assumed to be identical in the two cases) was restricted to 0.12 m . The conversions obtained in these two reactors, as a function of expanded bed height H , were calculated using equation (24) and are shown in Figure 7. The enormous influence of the scale of operation is evident on examination of Figure 7; for example to achieve 95% conversion in the pilot scale unit, an expanded bed height of 5.8 m is sufficient whereas in the commercial scale unit an expanded bed height of 10.2 m is required to achieve the desired 95% conversion level. It is interesting to note that the Shell Chlorine Process was designed for 95% conversion level and had an expanded bed height of 10 m , pointing to a good appreciation of the scale-up problems with fluid beds.

CONCLUDING REMARKS

Using the Darton bubble growth model, the Werther rise velocity correlation and the Davidson model for

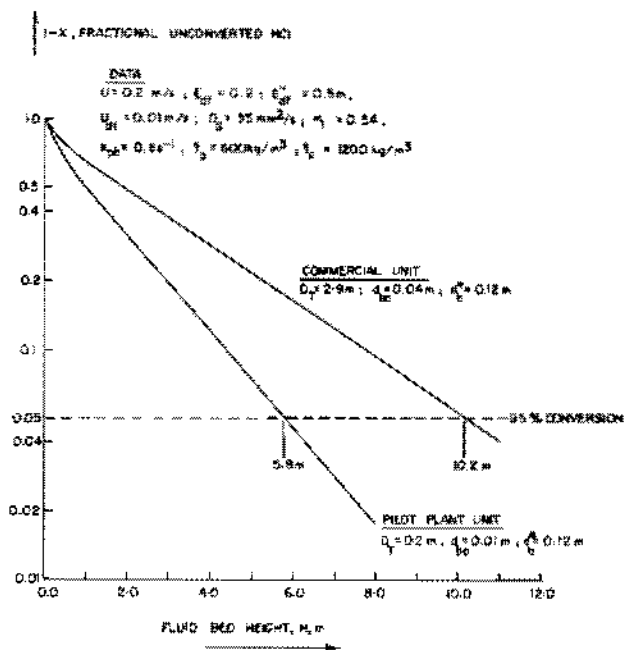


Figure 7. Influence of fluid bed diameter on the conversion achieved in the fluid bed process for oxidation of HCl.

interphase mass transfer, we have assembled together a usable model for simulation and design of fluidized bed reactors. The results of the model simulations for the air oxidation of HCl have highlighted the strong influence of bubble properties, especially the equilibrium bubble size, on the fluid bed performance. It is recommended that for design and scale-up purposes of new processes, the important parameters such as d_{b0} , d_b^* and U_{df} be determined in cold flow experiments (dynamic gas disengagement) in columns of sufficiently large size say greater than 0.6 m .

SYMBOLS USED

a_1, a_2	parameters defined by equation (25) [—]
a'	interfacial area per unit volume of gas dispersed in the form of bubbles [$\text{m}^2 \text{m}^{-3}$]
b_1, b_2, b_3	parameters defined by equation (25) [—]
d_b	diameter of a sphere having the same volume as the bubble in a fluidized bed [m]
d_{b0}	diameter of the bubble formed at the distributor plate, $h = 0$ [m]
d_b^*	maximum stable bubble size, attained at a height h^* above the distributor plate [m]
\bar{d}_p	mean particle size [m or μm]
D_{ax}	axial dispersion coefficient of the dense phase in a fluidized bed [$\text{m}^2 \text{s}^{-1}$]
D_0	molecular diffusion coefficient of the gaseous diffusing species [$\text{m}^2 \text{s}^{-1}$]
D_T	diameter of fluidized bed [m]
f	fraction of total reactor occupied by the dense phase gas, given by equation (17)
g	gravitational acceleration [9.81 m s^{-2}]
h	height of fluidized bed measured above the distributor [m]
h_0	height parameter characterizing the distributor, defined by equation (2) [m]
h^*	height above the distributor at which the bubbles attain their maximum stable bubble size d_b^* [m]
H	height of expanded fluidized bed [m]

$k_g a'$	volumetric mass transfer coefficient for bubble-to-dense phase, transfer, defined per unit volume of dispersed bubbles [s^{-1}]
k_{rb}	first order reaction rate constant, defined per unit volume packed bed volume (m^3 reacted) (m^3 packed bed) $^{-1} s^{-1}$
N_1, N_2, N_3	parameters defined by equations (28) [-]
NMU	number of mixing units, defined by equation (15) [-]
NTU	number of mass transfer units, defined by equation (11) [-]
NRU	number of reaction units, defined by equation (19) [-]
$[Q]$	matrix with elements given by equation (27) [-]
U	superficial gas velocity [$m s^{-1}$]
U_{df}	velocity (based on column cross-sectional area) of gas flowing through the dense phase [$m s^{-1}$]
V_b	absolute rise velocity of bubbles [$m s^{-1}$]
x	mole fraction of reactant species A [-]
x'	mole fraction of reactant in dilute phase [-]
x''	mole fraction of reactant in dense phase [-]
x_{in}	mole fraction of reactant in entering gas [-]
x_{out}	mole fraction of reactant in gas leaving the reactor [-]

Greek Letters

α_1	constant in Darton's bubble growth correlation, equation (1); $\alpha_1 = 0.54$
α_2	constant defined by equation (9c)
α_3	constant defined by equation (10b)
α_4	constant defined by equation (10b)
α_5	constant defined by equation (14c)
α_6	constant defined by equation (14d)
ϵ	expansion of fluidized bed with respect to settled bed [-]
ϵ_b	bubble phase hold-up as fraction of total fluid bed volume [-]
ϵ_{df}	expansion of dense phase with respect to settled bed [-]
ϵ_{df}'	void fraction of the dense phase [-]
λ	roots of the cubic equation (26) [-]
ν	fraction of gas flowing through the bubble phase, equation (12) [-]
ξ	fractional height, $\xi = h/H$ [-]
ρ_b	bulk density of particles [$kg m^{-3}$]
ρ_p	particle density [$kg m^{-3}$]
ϕ	Werther rise velocity constant, defined by equation (5) [-]
ϕ_1, ϕ_2	constants given by equation (6) [-]
χ	fractional conversion [-]

Superscripts

-	denotes integral height-averaged value
'	refers to dilute or bubble phase
''	refers to dense phase

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