SIMULATION OF BUBBLE POPULATIONS
IN A GAS FLUIDIZED BED

B H SHAH,† D RAMKRISHNA‡ and J D BORWANKER
Indian Institute of Technology, Kanpur, U P 208016, India

(Received 29 March 1976, received for publication 19 August 1976)

Abstract—The dynamics of bubble populations in a gas fluidized bed have been analyzed using a simulation technique due to the authors[11, 12] It is shown that small bubble populations arising from progressive coalescence may lead to inherent fluctuations which may be considerable Evidently, such fluctuations could manifest in conversions in fluidized bed reactors The results obtained were based on a model due to Argynou, List and Shnnar[1]

INTRODUCTION
Gas fluidized beds are of considerable importance to chemical engineers in view of their wide application to catalytic reactors The modeling of such reactors has been burdened by several complex features of their behavior so that a satisfactory description of gas fluidized beds has not been available Indeed a truly versatile quality is perhaps a presumptuous prescription for the model of a fluidized bed because of the diverse nature of the complicating factors Thus the normal complexities characteristic of homogeneous and packed bed tubular reactors are augmented by those which arise from the rapid random movement of the particle phase and the appearance of a "bubble phase" with relatively lean concentrations of suspended particles It is nevertheless useful to evaluate the isolated effects of some of the complexities even qualitatively if not quantitatively In the present work, we address ourselves to the dynamics of bubble populations, which originate at the distributor plate at the base of the bed and during their ascent progressively agglomerate to form bubbles of increasing sizes Argynou, List and Shnnar[1] have been the first to analyze bubble populations in a fluidized bed and to make an experimental evaluation of the same These authors employed the population balance framework of Hubert and Katz[2] incorporating a suitable agglomeration frequency to obtain the bivariate number density of bubbles as a function of bubble size (volume) and bed height They also used the bubble velocity expression in terms of bubble volume proposed by Rowe and Partridge[3] based on their experiments with single bubbles Orcut and Carpenter[4] have also investigated bubble coalescence experimentally using a single pulsed injector and could represent their results by a simulative technique which generated single bubbles of discrete sizes according to a Poisson distribution at the injector site More recently, Johnsson, Clift and Grace have used a simulative approach to predict bubble size distributions in a two-dimensional fluidized bed[5]

The analysis of Argynou et al[1] appeared reasonable over bed heights within which the bubble population had not depleted to particularly small values This is of course to be anticipated since the population balance equation employed by Argynou et al assumed that the sizes of the various bubbles were uncorrelated and the rate of coalescence between bubbles of volumes say v and v' at any position z was proportional to the numbers of bubbles of volumes v and v' respectively That particle states may be correlated in an agglomerative process is now recognized[6 10] Correlation between particle states throws an entirely different perspective into the analysis, since the model equations become an ascending hierarchy of equations in product densities[8] although when the initial number of particles is known, the set of equations is closed Ramkrishna, Shah and Borwanker[10] have demonstrated the development of correlation between particle states in an agglomerative process in which no correlation was assumed to be present between particle states in the initial population Thus the nature of the agglomeration frequency has a pronounced effect on the development of such correlations Furthermore, they showed that for small populations, fluctuations about average values may be of considerable magnitude, the "smallness" or "largeness" of a population was largely determined by the nature of the agglomeration kernel

The possibility of fluctuations arising from small bubble populations has far-reaching implications Thus there may appear as a result, fluctuations in the reactor performance, which could not obviously be described by a deterministic model of the bed Whether bubble populations are actually small enough in a fluidized bed for fluctuations to be important is of course a question to be answered It is the aim of this paper to incorporate the coalescence frequency employed by Argynou et al[1] with a slight modification, which renders it somewhat more realistic, into the more rigorous analysis of Ramkrishna et al[10] However, since the hierarchy of product density equations is computationally more difficult to solve, numerical solutions are obtained by a simulation technique, also due to the present authors[11]
THE MODEL

The situation of interest is a freely bubbling gas fluidized bed, which occurs when the superficial velocity of the gas is increased beyond the minimum fluidization velocity. The bubbles which are formed at the base of the bed are presumed to coalesce randomly as they ascend through the bed. Orcutt and Carpenter [4] consider only vertical coalescence between bubbles, that is, bubbles along any vertical row coalesce when a succeeding bubble catches up with the one above it. Johnsson et al. [5], on the other hand, consider a two-dimensional bed in which the two velocity components were both accounted for, coalescence occurred when bubble locations overlapped the bubble sites and sizes at the distributor plate were both allowed to vary randomly. However, a three-dimensional model promised by Johnsson et al. [5] in a forthcoming publication would of course labor to describe all three velocity components and record coalescence between bubbles in overlapping positions, any randomness in the system arising at the distributor plate where bubble sites and sizes would vary.

The model of Argyrou et al. [1], on which the present work is based, however takes a different perspective of the problem. Bubble locations are described by solely their vertical co-ordinates,‡ lateral motions are not explicitly accounted for but the resulting inability to identify exactly overlapping bubbles which can coalesce is then compensated for by the use of a coalescence frequency or a transition probability function for coalescence Argyrou et al. [1] set the coalescence frequency equal to zero for bubbles at different bed heights. We introduce a minor modification, which is self-evident from the pictorial representation in Fig. 1. Thus if $q(v, z, v', z')$ is the transition probability that a bubble of volume $v$ located at $z$ (at time $t$) will coalesce with another bubble of volume $v'$ located at $z'$, during the time interval $t$ to $t + dt$, then we may write

$$q(v, z, v', z') = \begin{cases} 0, & |z - z'| > d(v, v') \\ \frac{k_3}{k_3(v^{1/3} + v'^{1/3})^2}, & |z - z'| \leq d(v, v') \end{cases} \tag{1}$$

where

$$d(v, v') = \frac{1}{2} \left( \frac{v}{k_3^{1/3}} + \frac{v'}{k_3^{1/3}} \right) \tag{2}$$

‡The vertical co-ordinate of a bubble is that of its center

†It has been assumed that coalescence conserves the volumes of the coalescing bubbles although Johnsson et al. [5] indicate an approximate 10–15% increase in the volume.

$$Z = k_1 v^{1/6} \tag{3}$$

which carries with it the constraint that the fluidization velocities be small. Although entrapment of gas can change the volume of a given bubble, we assume such effects to be negligible.

The expected population density $f_i(v, z, t)$ must satisfy the equation (see for example [8–10])

$$\frac{\partial}{\partial t} f_i(v, z, t) + \frac{\partial}{\partial z} \left[ k_3 v^{1/3} f_i(v, z, t) \right]$$

$$= N f_i(v, z, v', z') \frac{\partial}{\partial z} \delta(z - L)$$

$$+ \int_{v/2}^{v} dv' \int_{-d(v-v')}^{d(v-v')} d(z') \delta(z - L)$$

$$\times f_i(v - v', z, v', z', t) dz'$$

$$+ \int_{v/2}^{v} dv' \int_{-d(v-v')}^{d(v-v')} d(z') \delta(z - L)$$

$$\times f_i(v - v', z, v', z', t) dz'$$

$$- \int_{v/2}^{v} dv' \int_{-d(v-v')}^{d(v-v')} k_3 \left( \frac{v - v'}{k_3} \right)^{1/3} \left( \frac{v'}{k_3} \right)^{1/3} f_i(v, z, v', z', t) dz' \tag{4}$$

where $f_i(v, z, v', z', t) dv \, dz \, dv' \, dz'$ represents the joint probability that at time $t$ there is a bubble of volume $v$ and $v + dv$ located between $z$ and $z + dz$ and another bubble of volume $v'$ and $v' + dv'$ located between $z'$ and $z' + dz'$. In deriving eqn (4) one must recognize that the coalesced bubble has been assigned the position of the larger of the two bubbles.

![Coalescence model](image-url)
before coalescence. Indeed eqn (4) must be supplemented by equations for the higher order product densities such as those obtained by Ramkrishna et al [10]. However we do not present these equations here since our approach is not one of obtaining solutions to the simultaneous equations comprising (4) and those in the higher order densities.

The first term in the right hand side of eqn (4) pertains to entering bubbles with

\[ N_f \, dt = Pr\{ \text{a bubble enters the bed at } z = 0 \text{ between } t \text{ and } t + dt \} \]  

(5)

and

\[ \phi(v) \, dv = Pr\{ v < \text{Bubble volume} < v + dv | \text{a bubble has entered} \} \]  

(6)

while the second term refers to the exiting bubbles at \( z = L \), where \( L \) is the height of the bed.

As pointed out earlier, the solution of eqn (4) in conjunction with the equations in the higher order densities is a difficult task and will not be pursued here. Instead, we approach the problem through a simulation technique due to Shah, Borwanker and Ramkrishna [11]. We are interested in the steady state behavior of the bed, the simulation by its very nature however involves starting from suitable initial conditions and evolving to the steady state through a transient. In order that the transient be short lived, the initial condition was picked to be the experimentally observed steady state bubble size and height distributions of Argyrrou et al [1].

**Simulation Algorithm**

The simulation technique of Shah et al [11, 12] has the distinct feature of being free from arbitrary discretization of the time interval. Instead, the evolution of the process is characterized by quiescence intervals, which are periods, during which the integrity of every particle in the population is preserved. In the present context, a quiescence interval is one during which no bubble loses its identity through coalescence with another, or no new bubble appears by entrance at the base. The population of interest is that contained within the bed, so that those bubbles, which have exited the bed do not account for the quiescence interval. The quiescence interval at any stage is conditional on the prevailing (known) state of the population. Probability distributions can be derived exactly for this interval of quiescence for any given particulate system. Random numbers may be generated following the derived distribution function, to represent sample realizations of the quiescence intervals.

Each simulation run is typified by the following steps:

The initial condition is fixed by the measured height distribution of bubbles with the size of each bubble at height \( z \) equal to the measured average bubble volume obtained by Argyrrou et al [1]. The quiescence interval distribution (to be subsequently identified) is then known. A random number is generated which realizes the quiescence interval during which bubble sizes are assumed to be invariant and their positions can be updated from the kinematics of bubble motion expressed by (3). At the end of the quiescence interval, it is of course certain that either a new bubble has entered or a coalescence event has occurred. The next step is to calculate the probability distribution for the two events bubble entry and any one coalescence out of the several coalescible pairs. When this is known a random number generated will realize one of the two events the subsequent step would depend upon whether a bubble entry took place or a coalescence event occurred. If a bubble entry took place, the size of the bubble will be generated by a random number, which has the probability density \( \phi(v) \), if a coalescence event occurred, then from the probability distribution for the specific coalescible pairs one can realize a particular pair by generating a suitable random number. In either case, the state of the population, which consists in identifying every bubble size and position will be known at the end of the quiescence interval. It should now be clear how a new quiescence interval can be generated and an entire "sample path" of the process can be generated over a specified period of time. Averages and fluctuations about averages can then be calculated using several sample paths generated by repeated simulations. What remains is the identification of the various probability distribution functions.

Let the state of the system be represented by \( A_i = [z_i, v_i, i = 1, 2, \ldots, N(t)] \), where \( z_i \) and \( v_i \) are respectively the height of the center and volume of the \( i \)th bubble and \( N(t) \) is the total number of bubbles in the whole bed. The determination of the quiescence interval requires the identification of the coalescible pairs. From eqn (1), we may regard the \( i, j \)th pair as coalescible if

\[ |z_i - z_j| = \frac{1}{2} \left[ \left( \frac{v_i}{k_1} \right)^{1/3} + \left( \frac{v_j}{k_1} \right)^{1/3} \right] \]

We denote the number of coalescible pairs by \( N_c \). The chance of coalescence between the \( i, j \)th pair in a small time interval \( dt \) is \( q(v_i, v_j) \, dt \), where \( q \) is given by eqn (1). The probability distribution of the interval of quiescence depends upon the probability that none of the \( N_c \) coalescible pairs coalesce and the probability that no bubble enters the bed during that interval. The value of \( N_f \) may be fixed by recognizing that the entering bubble volumes must sum to that volume of gas which is in excess of the minimum fluidization velocity \( U_o \). Thus

\[ N_f \int_0^\infty \phi(v) \, dv = \frac{\pi D^2}{4} (U - U_o) \]  

(7)

where \( U \) is the superficial gas velocity. If \( v_c \) is the average volume of entering bubbles, then (7) may be rewritten as

\[ N_f = \frac{\pi D^2 (U - U_o)}{4v_c} \]  

(8)

For lack of sufficient information about \( \phi(v) \) we assume

\[ \phi(v) = \frac{1}{(v_c^2)^{1/3}} \]
that all entering bubbles have volume \( v_a \), i.e., \( \phi(v) = \delta(v - v_a) \) Now the probability that either a bubble enters the bed or any one of the \( N_c \) coalesceable pairs coalesce during the time interval \( t \) to \( t + dt \) is \( (N_f + Q) dt \), where

\[
Q = \sum_{k=1}^{N_c} q(v_a, v_b)
\]

(9)
in which the \( k \)th coalesceable pair of bubbles has volumes \( v_a \) and \( v_b \). It is then readily shown[14] that the cumulative distribution function for the quiescence interval \( T \), i.e., \( F_T(T|A_t) = Pr\{T \leq \tau|A_t\} \) is given by

\[
F_T(T|A_t) = 1 - \exp \left[-(N_f + Q)\tau\right]
\]

(10)

To identify whether at the end of the quiescence interval, a bubble entry or a coalescence event had occurred we devise an indicator random variable \( I \), which has a value +1 if an entry has occurred and -1 if a coalescence event has occurred. It is easily verified that

\[
Pr\{I = 1|A_t, T\} = \frac{N_f}{N_f + Q}
\]

(11)

\[
Pr\{I = -1|A_t, T\} = \frac{Q}{N_f + Q}
\]

(12)

The advantage of the indicator random variable \( I \) is that the population at \( (t + T) \), i.e., \( N(t + T) \) can be written as \( N(t) + I \). It remains now to identify the coalescing pair, given that a coalescence event has occurred if \( u \) is another indicator random variable which can take on integral values between 1 and \( N_c \), \( u = r \) signifying the coalescence of the \( r \)th pair, then clearly

\[
Pr\{u = r|A_t, I = -1\} = \frac{q(v_a, v_b)}{Q}
\]

(13)

\( \dagger \)It is rather important to realize here that the number of coalesceable pairs does not remain strictly constant during a quiescence interval. This is because bubbles of unequal sizes have unequal velocities and the resulting relative velocities will change their distance of separation. However the error introduced by assuming constancy of \( N_c \) is rather small because the relative velocities from a \( v^{10} \) dependence are not very significant.

Thus the simulation of the fluidized bed may be represented by the sequence of random variables \( \{T_n, I_n, u_n\} \) \( n = 1, 2, \ldots \). The quiescence interval \( T \) can be generated using (10), eqns (11) and (12) may be used to generate \( I \), while (12) generates \( u \).

The simulation was also carried out using deterministic entry of bubbles, i.e., bubbles of volume \( v \) enter at regular intervals. Thus bubbles may enter the bed at times \( t_0, t_1, t_2, \ldots \), where

\[
t = t_{n-1} + \frac{1}{N_f}
\]

(14)

For this situation, the interval of quiescence at any instant \( T \) may be generated according to the distribution function

\[
F_T(T|A_t) = 1 - \exp \left[-Q\tau\right]
\]

(15)

The simulation proceeds as before save for a slight modification. If at any time \( t \) such that \( t_{n-1} \leq t \leq t_n \), it is found that

\[ t + T \geq t, \]

then the state of the system is advanced to \( t \), adding a new entering bubble at time \( t \). A coalescence event is simulated if \( t + T < t \).

RESULTS OF SIMULATION

The simulation was performed for random and deterministic entries of bubble for two different values of the ratio \( k_2/k_1 = k \). From the simulation results the bubble height and volume distributions were determined. Also the average number of bubbles in small slices of the bed were found along with the fluctuations about the average. The parameters of the bed, which were taken from the work of Argyrou et al [1], are listed in Table 1, specifically the parameters have been lifted from Fig 16 of Argyrou et al [1], which represents the results for a cracking catalyst with average solids size of 59 \( \mu \)m, solids density 55 lbm/ft\(^3\) and bulk density 32.5 lbm/ft\(^3\).

The value of \( k \) was determined by Argyrou et al [1] to be 0.026 in \(-3/2\) from their experimental results. Besides this value, simulations were performed for \( k = 0.26 \) in \(-3/2\).

<table>
<thead>
<tr>
<th>Table 1</th>
<th>The values of the fluidized bed parameters used in the simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \bar{v}_0 ), ft/sec</td>
</tr>
<tr>
<td>2</td>
<td>( \bar{v}/\bar{v}_0 )</td>
</tr>
<tr>
<td>3</td>
<td>( k_1 ), in (-3/2)</td>
</tr>
<tr>
<td>4</td>
<td>( k_2 ), in (1/2)/sec</td>
</tr>
<tr>
<td>5</td>
<td>( k_3 )</td>
</tr>
<tr>
<td>6</td>
<td>Maximum bed height, in</td>
</tr>
<tr>
<td>7</td>
<td>Minimum bed height at which the volume measurements were made, ( \tau_{\text{min}} ), in</td>
</tr>
<tr>
<td>8</td>
<td>Diameter of the bed, in</td>
</tr>
<tr>
<td>9</td>
<td>Volumes of the entering bubbles at 5 in bed height, in (^3)</td>
</tr>
</tbody>
</table>
Simulation of bubble populations in a gas fluidized bed

As mentioned earlier, the steady state is simulated necessarily from initial conditions, which are non-steady state situations. However, little transient periods were involved and steady states were attained quite rapidly, since the initial states were picked from the measured values of Argyrou et al. The approach of the average total number of bubbles $\bar{N}(t)$ to steady state values is shown in Fig. 2.

Table 2 displays the slicing of the bed within which the average number of bubbles and fluctuations about the average were determined.

Figures 3 and 4 show the estimates of the average number of bubbles $\bar{N}_n$ in the $n$th slice and also the percent coefficient of variation in the number $(\sigma N_n/\bar{N}_n) \times 100$, for $t = 0.25$ and $t = 0.50$ respectively. The latter is more representative of the steady state, $k$ has been 0.26 m$^{-3/2}$.

Both figures show the decrease in the average number of bubbles with bed height, which is as it should be. The more interesting feature however is the coefficient of variation, which increases at first and then diminishes towards the top of the bed with progressive coalescence.

![Fig 2 Simulation results of transients to steady state](image)

![Fig 3 Average number of bubbles and per cent fluctuation about average as a function of height along bed at $t = 0.25$ sec. Random bubble entry $k = 0.26$ m$^{-3/2}$](image)

<table>
<thead>
<tr>
<th>Slice No</th>
<th>Height, in</th>
<th>Slice Thickness, in</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>50</td>
<td>1.5</td>
</tr>
<tr>
<td>2</td>
<td>65</td>
<td>1.5</td>
</tr>
<tr>
<td>3</td>
<td>80</td>
<td>1.5</td>
</tr>
<tr>
<td>4</td>
<td>95</td>
<td>1.6</td>
</tr>
<tr>
<td>5</td>
<td>111</td>
<td>1.6</td>
</tr>
<tr>
<td>6</td>
<td>127</td>
<td>1.5</td>
</tr>
<tr>
<td>7</td>
<td>142</td>
<td>1.5</td>
</tr>
<tr>
<td>8</td>
<td>157</td>
<td>1.5</td>
</tr>
<tr>
<td>9</td>
<td>172</td>
<td>1.6</td>
</tr>
<tr>
<td>10</td>
<td>188</td>
<td>1.6</td>
</tr>
<tr>
<td>11</td>
<td>204</td>
<td>1.5</td>
</tr>
<tr>
<td>12</td>
<td>219</td>
<td>1.5</td>
</tr>
<tr>
<td>13</td>
<td>234</td>
<td>1.5</td>
</tr>
<tr>
<td>14</td>
<td>249</td>
<td>1.6</td>
</tr>
<tr>
<td>15</td>
<td>265</td>
<td>1.6</td>
</tr>
<tr>
<td>16</td>
<td>281</td>
<td>1.5</td>
</tr>
<tr>
<td>17</td>
<td>296</td>
<td>1.5</td>
</tr>
<tr>
<td>18</td>
<td>311</td>
<td>1.5</td>
</tr>
<tr>
<td>19</td>
<td>326</td>
<td>1.6</td>
</tr>
<tr>
<td>20</td>
<td>342</td>
<td>1.6</td>
</tr>
</tbody>
</table>

Table 2 Heights and thicknesses of the slices of bed in which the number of bubbles were determined.
Figures 5 and 6 show the estimates of the average cumulative number distribution of bubbles in bubble volume and height \( \beta(z, v, t) \) at two different times. Figure 7 is more representative of the steady state. These figures also provide information about the bubble size and reflect quantitatively the obvious fact that bubble sizes must increase with bed height.

Figures 7 and 8 show the steady state results for \( k = 0.026 \text{ m}^{-3/2} \). The trends in the number of bubbles in various bed slices are those for \( k = 0.26 \). The significant difference is that the percent coefficient of variation is now practically negligible throughout the bed. Thus, in part, explains why the population balance model of Argyriou et al. performed as well as it did. Our calculations with \( k = 0.26 \) demonstrate that this success of the population balance model is not always guaranteed.

It is easy to see in the light of our previous publication[10], why the value of \( k \) has such a profound effect on the fluctuations in the bed. The larger value of \( k \) promotes rapid coalescence leaving a relatively smaller population of bubbles in the bed. Smaller populations can give rise to fluctuations that are often considerable. Also, particle states become strongly correlated so that the population balance model becomes inadequate. The value of \( k \) has much to do with the bed geometry, distributor plate, characteristics of the fluidized solids, gas velocity.
Simulation of bubble populations in a gas fluidized bed

Steady State Operation

$N_\infty = 130 \quad k = 0.026 \text{ m}^{3/2}$

$S = 10 \quad t = 0.01 \text{ sec}$

Random Entry

Determination of Fluidized Bed

Fig. 8 Average number of bubbles and per cent fluctuation about average as a function of height along bed at $t = 0.02 \text{ sec}$

etc., if the coalescence frequency expression (1) is not acceptable, the preceding statements hold for any substitute expression also

CONCLUSIONS

If the rates of coalescence of bubbles in a fluidized bed are sufficiently high, the fluctuation in bubble populations are found to reflect on such quantities as reaction conversions in fluidized bed reactors

The publications of Orcutt and Carpenter[4] and Johnsson et al [5] seem to indicate a trend towards stochastic modeling of fluidized beds Indeed stochastic features would manifest if bubble formations at the distributor plate occur randomly Bubble coalescence itself was treated deterministically in the cited works since bubble motion has been assigned deterministic kinematics The present work, however is to be distinguished from the above, for although the vertical climb has been assumed to be deterministic, the kinematics of bubble motion with respect to the two other components has been assumed to be random, this implication arises from the fact that a transition probability function has been assigned for coalescence Thus superimposed on the randomness associated with bubble entry is the randomness in bubble coalescence Whether the combination produces a randomly behaving bed is what has been the focus of our attention Indeed our conclusion is that if bubble coalescence is sufficiently rapid to produce small bubble populations a stochastic treatment is indispensable

NOTATION

$A_t$ state of population of bubbles at time $t$

$D$ bed diameter

$d$ maximum distance between coalescible bubbles (a function of bubble volumes)

$E$ expected value

$F_r$ cumulative distribution function for random variable $T$

$I$ indicator random variable defined above eqn (11)

$k_1$ constant in eqn (3)

$k_2$ constant in eqn (1)

$k_3$ shape factor in eqn (3)

$k, k_2/k_1$

$L$ height of bed

$N(t)$ number of bubbles at time $t$ in the entire bed

$N_c$ number of coalescible bubble pairs in the bed

$N_f$ transition probability function for bubble entry

$P_r$ probability

$Q$ defined by eqn (9)

$q$ coalescence frequency (a function of bubble volumes and heights, given by eqn (1)

$S$ number of simulations

$T$ quiescence interval

$t$ time

$U$ superficial gas velocity, $U_a$ minimum fluidization velocity

$u$ indicator random variable defined above eqn (13)

$v$ bubble volume $v_e$ average volume of entering bubbles

$z$ vertical distance along bed Height of bubble

$Z$ bubble velocity

Greek symbols

$\beta$ joint cumulative number distribution of bubbles in bubble volume and height

$\phi$ probability density of volumes of entering bubbles

$\sigma$ standard deviation

$\tau$ typical value of quiescence interval

$\hat{}$ above a symbol means estimated value

REFERENCES


