STOCHASTIC MODEL FOR FLUIDIZATION

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INTRODUCTION

Fluidized beds are among those basic reactors that have been used extensively for various applications in the process engineering industry. In spite of this, and as a result of the complex motion of fluids and particles inside the beds, still more information is needed to understand the transportation of particles inside the bed. During the last decade, a number of different methods, such as X-ray and radioactive tracing techniques, have been used to monitor the dynamics of particles inside fluidized beds.

In this paper we investigate particle transport in a batch fluidized bed reactor using an advanced technique, Positron Emission Tomography (PET). The results from this new tracing technique are presented by van der Zwan (1). This method, made possible by cooperation with Groningen University Academic Hospital (AZG), offers the possibility of following the dispersion through the fluidized bed of a pulse of marked particles in 3-D in real time. The experiments were performed by labeling particles with ^{18}F isotope and tracking them by a medical PET camera in a period of time.

Dehling *et al.* (2) proposed to model the particle transport in a fluidized bed reactor by a stochastic process for an individual particle. Also stochastic models have been successfully constructed to model the particle dynamics in different types of gas-solid fluidized bed reactors e.g., slugging fluidized beds (3) and bubbling fluidized beds with baffles (4). This microscopic approach has the clear advantage over traditional PDE models obtained from conservation equations, in that models for the motion of individual particles are often easier to formulate and intuitively more convincing. At the same time, one can recover traditional PDE models, such as Fokker-Planck equations for the probability density of the particles in the stochastic process.

Dehling *et al*. (2) investigated residence time distributions in continuous fluidized beds using stochastic modeling. They applied their technique to various experimental setups and showed that the RTD curves could be predicted surprisingly well.

The stochastic modeling approach of Dehling *et al*. (2) also allows computation of the particle density inside the reactor. The data obtained by van der Zwan (1) using the PET technique allow for the first time a comparison with experimentally obtained particle density. To validate the models, and model concepts, a number of different experiments have been performed using different tracing techniques, such as sectioning the bed and analyzing the distribution of a colored tracer, taking images by high speed camera and using X-ray techniques. The data gains from these tracing techniques, have been reported elsewhere.

Our stochastic models predict the position probability of a single particle. By the law of large numbers this reflects the behavior of a pulse of marked particles in the system. It is the goal of the present paper to analyze the particle density obtained in the PET experiments of van der Zwan (1) that are considered as a direct method and to compare them with theoretical predictions.

DESCRIPTION OF THE STOCHASTIC MODEL

This model is based on Dehling and Hoffmann's modeling concepts(2), for particle transport in bubbling fluidized beds based on a convection-diffusion process. In this paper we study a batch fluidized bed, where there is no inflow and outflow of the particles during the process. The motion of one particle is considered, and the transport processes are converted to transition probabilities between cells in a discretized bed, see Figure 2. The probability distribution for the particle's position as a function of time reflects the behavior of a radioactive particle. The model is based on Markov chains, such that the transition probability distribution of a single particle is independent of the past history of the system.

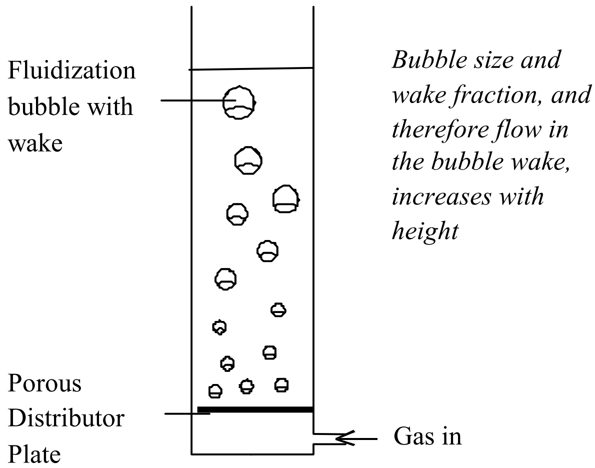

Figure 1. Sketch of a bubbling fluidized bed.

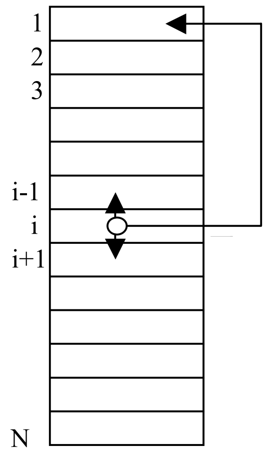

Figure 2. The discretized fluidized bed.

MODELING

In our discrete Markov model, the reactor is divided into N horizontal cells, and we model the particle's position at discrete times only. The cells are numbered as shown in Figure 2. The model calculates the probability distribution of the axial position of one particle as a function of time. The possible transitions are:

a) staying in the same cell
b) moving to the next cell
c) moving back to the previous cell
d) being caught up in a bubble wake and deposited at the top of the bed

We introduce parameters α_i, β_i and δ_i, with sum equal to 1, for the first three probabilities, conditionally on the particle not being caught up in a bubble wake, the latter probability being given by λ_i.

The transfer probabilities from cell i to cell j form a matrix, $\boldsymbol{Q}$, with the elements $q_{i,j}$. The transition probabilities for the interior of the reactor, *i.e.* for $2 \le i \le N-1$, are:

$$
\begin{aligned}
q_{i,i} &= \alpha_i(1-\lambda_i)\\
q_{i,i+1} &= \beta_i(1-\lambda_i)\\
q_{i,i-1} &= \delta_i(1-\lambda_i)\\
q_{i,1} &= \lambda_i
\end{aligned}
\tag{1}
$$

Regarding the boundaries, i.e., $i = 1$ and $i = N$;

$$
\begin{aligned}
q_{1,1} &= 1-\beta_1(1-\lambda_1),\\
q_{1,2} &= \beta_1(1-\lambda_1),\\
q_{N,N} &= 1-\delta_N(1-\lambda_N)-\lambda_N\\
q_{N,1} &= \lambda_N\\
q_{N,N-1} &= \delta_N(1-\lambda_N)
\end{aligned}
\tag{2}
$$

The probability distribution of the position of the particle at the n'th time step is given by the probability vector $\boldsymbol{p(n)}$, with elements denoted by $p(n,i)$.

Knowing $\boldsymbol{p(n\text{-}1)}$, one can find $\boldsymbol{p(n)}$ from:

$$
p(n,j) = \sum_{i=1}^{N} p(n-1,i)q_{i,j} \quad \textit{or in matrix notation :} \quad \boldsymbol{p(n) = p(n-1)Q} \tag{3}
$$

After n time steps, we obtain the formula for the probability distribution of position of the particle at time n in terms of its initial probability distribution:

$$
\boldsymbol{p}(n) = \boldsymbol{p}(0)\boldsymbol{Q}^n \tag{4}
$$

which $\boldsymbol{p}(0)$ is the initial condition of particle distribution in the reactor at time $t=0$.

MARKOV CHAIN MODEL

The model introduced above is a discrete one, but the transfer probabilities will be related to physical parameters describing the particle transport as continuous processes, following Dehling *et al.* (2). We call the time step ε and the cell width Δ. Letting ε and Δ go to 0, we obtain a discrete Markov chain approximation to the continuous process.

The vertical distance from the top of the reactor is denoted by x, i.e., $x = 0$ corresponds to the top and $x = 1$ to the bottom, and the convective axial velocity due to circulation by $v(x)$. The dispersion due to the disturbance by bubbles is denoted by a dispersion coefficient, $D(x)$. The rate of returns to the top of the bed is described by $\lambda(x)$. The parameters in the transition matrix are defined as follows:

$$
\delta_i = \frac{\varepsilon}{2\Delta^2}D(i\Delta) - \frac{\varepsilon}{2\Delta}v(i\Delta), \tag{5}
$$

$$
\beta_i = \frac{\varepsilon}{2\Delta^2}D(i\Delta) + \frac{\varepsilon}{2\Delta}v(i\Delta), \tag{6}
$$

$$
\alpha_i = 1-\delta_i-\beta_i, \tag{7}
$$

$$
\lambda_i = \varepsilon\lambda(i\Delta) \tag{8}
$$

Both the axial velocity due to circulation of particles as well as the return rate of particles are functions of the particle flow in the wake of rising fluidization bubbles. If Q_w denotes the wake flow and A the cross-sectional area of the bed, we have: $v(x) = \frac{Q_w(x)}{A}$ and $\lambda(x) = \frac{d}{dx}\left(\frac{Q_w(x)}{A}\right)$.

STATISTICAL ANALYSIS

In this section we look at the vertical particle displacement. We have investigated the mean square displacement of the particles $\sigma_t^2 := E(X_t - X_0)^2$ in the reactor as a function of time. For small times σ_t^2 should be approximately proportional to t, with the diffusion coefficient D as proportionality constant.

We can estimate σ_t^2 from the positions $X_t(k), k = 1, \ldots, K$, of all individual particles at time t by $\frac{1}{K}\sum_{k=1}^{K}(X_t(k) - X_0(k))^2$. In our experimental setup, all particles had the same vertical position x_0, so that the estimation becomes $\frac{1}{K}\sum_{k=1}^{K}(X_t(k) - x_0)^2$. Alternatively, if $x_i, i = 1, \ldots, N$, denote the z-coordinate of the center of the i-th cell, and ρ_i the fraction of particles in that cell, we can estimate σ_t^2 by $\hat{\sigma}_t^2 = \sum_{i=1}^{N}\rho_i(x_i - x_{i_0})^2$, where i_0 is the index of the cell that contained the pulse initially.

COMPARISON WITH EXPERIMENTS

Three different types of pulse experiments were carried out to study the dispersion of horizontal layers, initially positioned at the bottom, middle and top of the fluidized bed. In this paper, initial results for the top and middle layer experiments are compared with the model predictions. The experimental data for the top layer experiment are shown Figure 3 and Figure 4 shows a result from our model prediction.

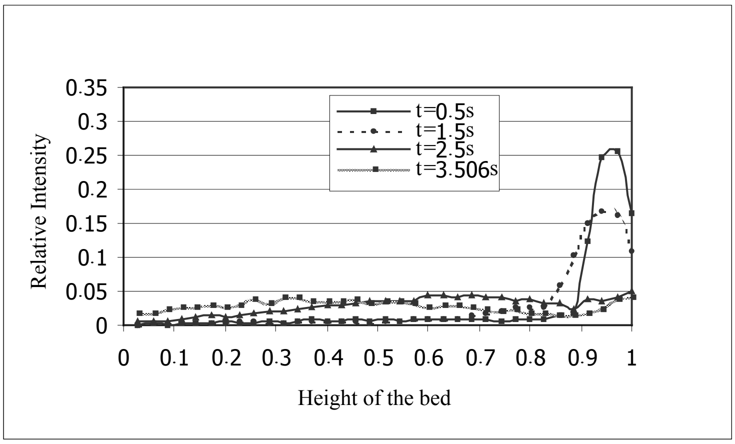

Figure 3. Graph of the experimental data for relative intensity as a function of normalized height (-) of the experiment with a layer in the top.

The particle flow in the wake phase as well as the dispersion coefficient have been computed in the same way as in Dehling *et al.* (2), building on the earlier work of Geldart (5), Hoffmann and Paarhuis (6) and Tanimoto *et al*.(7). Using these parameter values, our model predicts the densities given in Figure 4.

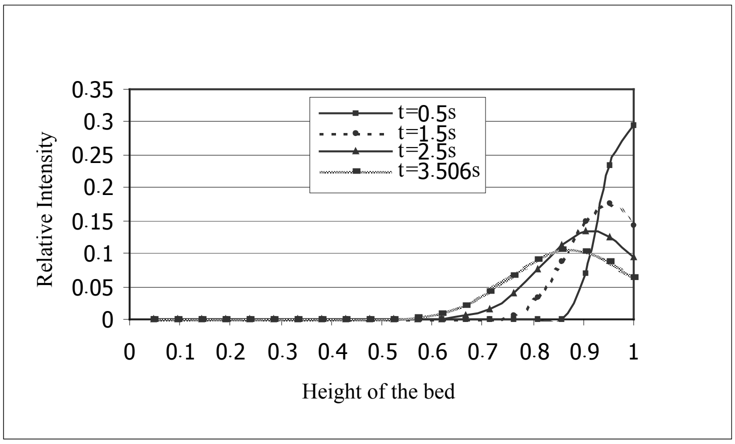

Figure 4. Graph of the model prediction for relative intensity as a function of height (-)of the experiment with a layer in the top.

Figures 3 and 4 show good agreement between the predicted and experimental data, the initial mixing of the layer into the bed is predicted quite well. Both the experimental results and the model predictions can be improved.

Figures 5 and 6 show experimental results and model predictions for the dispersion of a layer initially positioned in the middle of the bed. Also here the predictions are seen to agree with experiment.

Looking closely at the figures, however, it can be seen that the model predicts the peak to move slightly downwards while decreasing in height. The preliminary experimental data, while less clear, seem to indicate an upwards movement of the peak. Later results, which will be published separately and some of which are shown in (8), show a downwards movement of the peak as it is dispersing, in agreement with the model predictions in Figure 6.

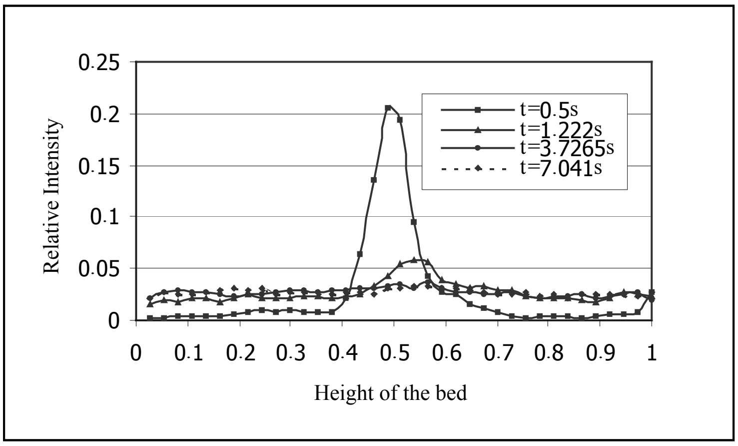

Figure 5. Graph of the experimental data for relative intensity as a function of height(-) of the experiment with a layer in the middle.

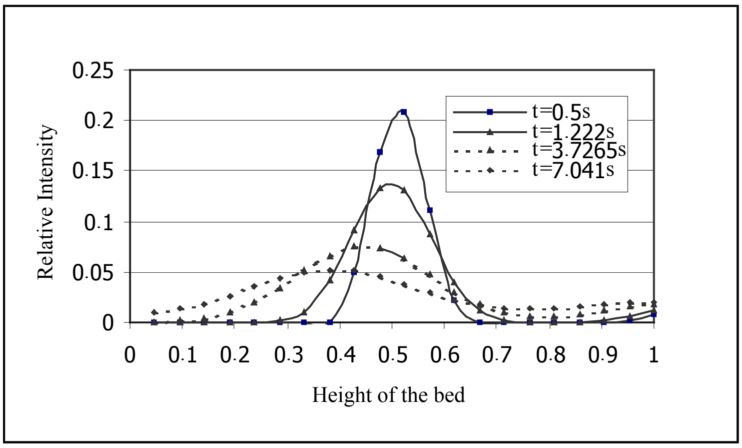

Figure 6. Graph of the model prediction for relative intensity as a function of height(-)of the experiment with a layer in the middle.

CONCLUDING REMARKS

Our model takes into account only one dimension so far. The detailed information we obtained from the PET technique can be used to further validate our model and to support expansion of it to two or three dimensions by studying the radial dispersion in the bed.

Our stochastic model is appealing as it is a simple and elegant approach. Another attractive feature is the ease with which models are formulated even for relatively complicated processes. We stress that this latter advantage does not depend on the scatter in the process results, but is present also for systems containing so many particles that they – by the law of large numbers –can be described effectively in a deterministic way.

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REFERENCES

(1) van der Zwan E (2001) *PET: A New Method for Analyzing Fluidized Beds*, Master thesis, Department of Chemical Engineering, University of Groningen, Groningen, The Netherlands.
(2) Dehling H G, Hoffmann A C and Stuut H W (1999) Stochastic models for transport in a fluidized bed. *SIAM J. Appl. Math. 60*, pp 337-358.
(3) Dechsiri C, Abanades J C, Dehling H G, Hoffmann A C and Wright P C (2000) A stochastic model for mixing and segregation in slugging fluidized beds. *Proc the 3rd European Fluidization conference*, Toulouse.
(4) Dechsiri C, Bosma J, Dehling H G and Hoffmann A C (2001) A stochastic model for mixing and segregation in fluidized beds with baffles. *Proc PARTEC 2001*, International Congress for Particle Technology,Nürnberg, march 2001.

(5) Geldart D (1972)The effect of particle size and size distribution on the behavior of gas-fluidized beds. *Powder Tech. 6,* pp 201-215.
(6) Hoffmann A C and Paarhuis H (1990) A study of the particle residence time distribution in continuous fluidized beds, *I.Chem.E.Sympos. Ser. 121,* pp.37-49.
(7) Tanimoto H S, Chiba S, Chiba T and Kobayashi H (1981) Jetsam descent induced by a single buble passage in three-dimensional gas-fluidized beds. *J. Chem. Eng. Of Japan, 14,* pp 273.
(8) Dechsiri C, van der Zwan, E, van de Wiel, F, Bosma J, Paans, A M J and Hoffmann A C (2002) Positron emission tomogrpahy (PET) for fluidization *Proc. World Congress in Particle Technology 4*, Sydney, July 2002.