Chapter 7

Interacting Particle Model for Segregation in Fluidized Beds

7.1 Introduction

In Chapter 3 to 6, transport phenomena in fluidized bed reactors have been studied with the help of models for the motion of a single particle. These models have also been used to predict the diffusion of a pulse of marked particles (see Chapter 4), assuming independence of the particles motion. This is justified as long as the proportion of marked particles is rather small, as was the case in all the experiments analyzed and described in Chapter 3 to 6. There our single particle model was very successful in predicting the results of the experiments.

When there is a sizable fraction of marked particles in the reactor, however, interaction among particles becomes relevant. The simple fact that no two particles can occupy the same location implies that there is an upper bound on the concentration of marked particles. In the earlier chapters, the problem of interaction was addressed in a rather ad hoc manner. This chapter then presents a study of a particle transport model that incorporates interaction effects in a fundamental way.

7.2 Particle Exchange Model for Diffusion

To present the essential ideas, we first investigate a model for only diffusion transport, and do not take the transport in the wake phase into account. Incorporating wake transport will be done in the following section. Moreover we concentrate in a batch fluidized bed which for modeling we divide vertically into $N$ horizontal layers (cells) of equal height. We assume that there are two types of particles in the reactor, say marked (jetsam) and unmarked particle (flotsam). For simplicity we assume that each cell holds exactly $K$ particles. So, in total the reactor contains $NK$ particles and we assume that $M$ of these are marked. We denote by $y_i(t)$ the number of marked particles in cell $i$ at time $t$. The state of our system at time $t$ is thus described by the vector $y_t := (y_1(t), \ldots, y_N(t))$. 
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The basic transport mechanism in our model is the exchange of particles between neighboring cells. In this exchange marked particles are preferentially chosen for downward transport and this will result in segregation of particles. Particle exchange starts by choosing a cell at random, its number denoted by \( i \), where \( i \in 1, \ldots, N - 1 \). We then choose one particle from cell \( i \) and one from cell \( i + 1 \) using a weighted probability distribution, and have these particles exchange positions. The particle selected from cell \( i \) is a marked particle with probability

\[
\frac{\alpha y(i)}{\alpha y(i) + K - y(i)} = \frac{\alpha y(i)/K}{\alpha y(i)/K + 1 - y(i)/K} = \frac{\alpha c(i)}{\alpha c(i) + i - c(i)}
\]

and unmarked with probability

\[
\frac{K - y(i)}{\alpha y(i) + K - y(i)} = \frac{1 - c(i)}{\alpha c(i) + 1 - c(i)}.
\]

In these formulae, \( c(i) \approx \frac{y(i)}{K} \) denotes the concentration of marked particles in cell \( i \) and \( \alpha \geq 1 \) is a constant governing the degree of preference for a marked particle to be chosen for downward transport. Observe that \( \alpha = 1 \) would imply that the particle is selected at random from among the \( K \) particles in cell \( i \).
Similarly, we assume that the particle chosen from cell $i+1$ for upward transport is marked with probability
\[
\frac{\beta c(i+1)}{\beta c(i+1) + 1 - c(i+1)},
\]
and unmarked with probability
\[
\frac{1 - c(i+1)}{\beta c(i+1) + 1 - c(i+1)},
\]
where $\beta \leq 1$ is again a weight factor.

The above defines a Markov process $\{Y_t \in \mathbb{N}_0 : \sum_{i=1}^{N} y(i) = M \}$ with parameter space $\mathbb{N}_0$ and state space $S = \{(y(1), \ldots, y(N)) : y(i) \in \mathbb{N}_0 : \sum_{i=1}^{N} y(i) = M \}$. This state space is too big to allow numerical calculations of particles densities as in our earlier models. In Figure 7.2 we show the concentration of marked particles after 1,000,000 iterations for a model with $N = 20$, $K = 400$, $M = 4,000$, $\alpha = 1.2$, $\beta = 0.8$ and a uniform initial distribution of marked particles. Convergence for a large number of cells is rather slow and more attention should be paid to find efficient algorithms.

### 7.3 Invariant Density for a Large Number of Particles

As the number of transitions increases, the distribution of the Markov process will converge to a steady state. This steady state distribution fluctuates around the infinite particle limit, and fluctuations decrease at $\frac{1}{\sqrt{K}}$ rate as we let the number of particles go to infinity, i.e. $N \to \infty, K \to \infty$ in such a way that $K/N \to \gamma \in [0,1]$. In what follows we will compute this infinite particle limit.

Still denoting the concentration of marked particles in cell $i$ by $c(i)$, we get in our model a transition from $y(i)$ to $y(i)+1$ if a marked particle from cell $i+1$ exchanges position with an unmarked particle from cell $i+1$. This event has probability
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\[
\frac{\beta c(i+1)}{\beta c(i+1) + 1 - c(i+1)} \cdot \frac{1 - c(i)}{\alpha c(i) + 1 - c(i)} \quad (7.1)
\]

Figure 7.2 Density of marked particles in a pure diffusion model with segregation obtained from 1,000,000 iterations with \(N=20, K=400, M=4000, \alpha=1.2, \beta=0.8\). The smooth curve is that found in Section 7.2 for this example.

In similar way, we get that a transition from \(y(i)\) to \(y(i)-1\) occurs with probability

\[
\frac{\alpha c(i)}{\alpha c(i) + 1 - c(i)} \cdot \frac{1 - c(i+1)}{\beta c(i+1) + 1 - c(i+1)} \quad (7.2)
\]

The event of no change in the distribution of marked particles occurs when either two marked or two unmarked particles exchange positions, and this has probability

\[
\frac{\alpha c(i)\beta c(i+1)(1-c(i))(1-c(i+1))}{(\alpha c(i) + 1 - c(i))(\beta c(i+1) + 1 - c(i+1))}.
\]

A steady state is reached if there is no drift, and this means that (7.1) and (7.2) must be equal. We thus arrive at the following condition,
\[ ac(i)(1 - c(i + 1)) = \beta c(i + 1)(1 - c(i)) \]

which can be rewritten as

\[ \frac{c(i + 1)}{1 - c(i + 1)} = \frac{\alpha}{\beta} \frac{c(i)}{1 - c(i)}. \]

This iteration can be solved explicitly by

\[ \frac{c(i)}{1 - c(i)} = \left( \frac{\alpha}{\beta} \right)^i \frac{c(0)}{1 - c(0)} = e^{\gamma_i \gamma_0}, \quad (7.3) \]

where \( \gamma_0 = \log \frac{c(0)}{1 - c(0)} \) and \( \gamma_1 = \log \frac{\alpha}{\beta} \). We can solve (7.3) explicitly for \( c(i) \) and get

\[ c(i) = \frac{e^{\gamma_0 + \gamma_1 i}}{1 + e^{\gamma_0 + \gamma_1 i}}. \]

If we consider the continuous limit obtained by letting the space discretization converge to zero, or equivalently \( N \to \infty \), the concentration of marked particles in the steady state becomes

\[ c(x) = \frac{e^{\gamma_0 + \gamma_1 x}}{1 + e^{\gamma_0 + \gamma_1 x}}, 0 \leq x \leq h, \quad (7.4) \]

where \( \gamma_0 \in \mathbb{R} \) and \( \gamma_1 \geq 0 \) are parameters.

If the average concentration of marked particles in the reactor is known, this puts a restriction on the parameters \( \gamma_0 \) and \( \gamma_1 \). Suppose the average concentration is \( C \), then we get
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\[
C = \frac{1}{h} \int_0^h c(x) dx = \frac{1}{h} \int_0^h \frac{e^{\gamma_0 x}}{1 + e^{\gamma_0 x}} dx \\
= \frac{1}{h\gamma_1} \log(1 + e^{\gamma_0 x}) \bigg|_{x=0}^{x=h} \\
= \frac{1}{h\gamma_1} \log \frac{1 + e^{\gamma_0 h}}{1 + e^{\gamma_0}}.
\]

We can solve this to get an explicit equation for \( \gamma_0 \). Via some calculations we find

\[
e^{\gamma_0 c} (1 + e^{\gamma_0}) = 1 + e^{\gamma_0} e^{\gamma_0 h}
\]

and thus

\[
e^{\gamma_0} = \frac{e^{\gamma_0 c} - 1}{e^{\gamma_0 h} - e^{\gamma_0}}
\]

from where we finally obtain

\[
\gamma_0 = \log \left( \frac{e^{\gamma_0 c} - 1}{e^{\gamma_0 h} - e^{\gamma_0}} \right).
\]

Figure 7.3 Invariant densities according to the pure diffusion model for average concentration \( C = 0.5 \) and \( \gamma_1 = 1 \) (solid line), \( \gamma_1 = 5 \) (dashed line), \( \gamma_1 = 10 \) (dash-dotted line) and \( \gamma_1 = 100 \) (dotted line)
In Figure 7.3 we have drawn graphs of the concentrations for the fixed average concentration of $C = 50\%$ and a variety of values of the parameter $\gamma_1$.

### 7.4 Comparison with Data

If we want to fit this model to the data, we can take logarithms on both sides of (7.3) and obtain

$$
\log \left( \frac{c(i)}{1-c(i)} \right) = \log \lambda + i \log \left( \frac{\alpha}{\beta} \right) = \gamma_0 + \gamma_1 i.
$$

This suggests determining $\gamma_0$ and $\gamma_1$ by a least squares linear regression of $\log \left( \frac{c(i)}{1-c(i)} \right)$ on $i$.

Comparing the data (see Figure 7.4) to our model prediction we find that the near constant concentration of marked particles at the top of the reactor cannot be well fitted by our model. We can interpret the fact that particles at the top of the reactor are almost perfectly mixed as a result of wake flow that will continuously transport particles from the bottom of the reactor to the top.

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**Figure 7.4 Comparison of jetsam particles in a fluidized bed reactor (Dechsiri, et al., 2001)**
7.5 Particle Model for Diffusion and Wake Flow

In this section we add wake flow to the model discussed in section 7.3. For the sake of simplicity, we assume that only particles in the bottom cell can move upwards in the wake flow. They are then deposited at the top of the reactor. As a result there is a downward flow of particles to fill the void left by the wake flow.

To put the wake flow and diffusion effects on the same scale, we set the basic time unit of the process to $N$ cycles of the exchange of particles between adjacent cells. Then on average every pair of cells has been chosen once during the time unit. After each such unit time, a Poisson number of particles is picked from the bottom cell, here each particle is with probability $\frac{y(N)}{K}$ marked and with probability $1 - \frac{y(N)}{K}$ unmarked. Denoting these numbers by $U$ and $V$ respectively and $W := U + V$, we have the following distributional properties:
\[ W \sim \text{Poisson}(\lambda) \]
\[ U \sim \text{Poisson}(\lambda \cdot \frac{y(N)}{K}) \]
\[ V \sim \text{Poisson}(\lambda (1 - \frac{y(N)}{K})) \]

and \( U, V \) are two independent random variables. These particles are then deposited at the top and the void left at the bottom induces a downward flow of particles. We model this downward flow as in section 7.1. Each of the \( W \) particles that move from cell \( i \) to cell \( i+1 \) is marked with probability \( \frac{ay(i)}{ay(i) + K - y(i)} \) and unmarked with probability \( \frac{K - y(i)}{ay(i) + K - y(i)} \). When applying this, one has to realize that the choice of particles that move influences the possible moves in neighboring cells so that the order is important. We start from \( i = N - 1 \) and go upward to \( i = 1 \).

7.6 References


Dechsiri, C., van der Wiel, Dehling, H.G., Hoffmann, A.C. and Paan, A.M.J., “Positron emission tomography applied to fluidization engineering” *Proceeding of*

