Further Refinements of a Stochastic Model for Particle Sedimentation in Fluids

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Abstract

The engineering sciences have long been interested in models describing the settling (or sedimentation) of particle ensembles in viscuous fluids. From a theoretical point of view sedimentation constitutes a two phase, many-body phenomenon with complex interaction and as such has proved to be quite inaccessible to modelling attempts with relevance in applications. A stochastic model was introduced by Pickard and Tory in 1977 and was subsequently revised and refined. In this paper we develop the stochastic model further and also present a satisfactory modelfitting procedure and parameter estimators based on transit times of sedimenting particles.

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0. Introduction.

In recent years, the Chemical Engineering community has become increasingly interested in models describing particle sedimentation in viscuous fluids. This interest reflects a need among engineers and hydrologists for a utilizable theory to handle this two-phase, many-body problem and contrasts sharply with the absence of such a theory.

By sedimentation here is meant the collection of phenomena arising in a two-phase solids-fluid system that evolves under the influence of gravity (and possibly other forces) from some initial state. In theoretical terms sedimentation constitutes a phenomenon in the domain of continuum mechanics and it is possible, at least in principle, to set up the equations of motion for all particles and fluid flows. However, since the number of particles involved is quite large the problem becomes very high dimensional and hence intractable.

Kynch (1952) has dealt with this intractability by introducing very restrictive simplifying assumptions. These assumptions allow to obtain solutions of the equations of motion <u>not</u> for individual particle trajectories but for averages of particle motion. In this sense Kynch's theory describes average ensemble behavior but cannot interpret the wealth of phenomena arising from the variability of particle behavior.

Section 1 will briefly review both the hydrodynamic approach and Kynch's theory.

Section 2 then gives a compact description of an updated version of a stochastic model for sedimentation. The basics of this model were first introduced by Pickard and Tory in 1977. It has since then been refined and undergone revision (see Pickard and Tory (1979, 1982, 1986)) and important work has been done recently (Hesse (1987)). The present author became involved in the project when he joined the Department of Statistics at Harvard University in 1984 to work with the late D. Pickard.

The present paper also addresses issues of modelfitting and parameter estimation and we present simple estimators for all relevant model parameters. These are based on recent solutions of first-passage time problems (Hesse (1990)) and allow to utilize existing extensive industrial data bases containing mostly transit times of particles in sedimentation.

In the stochastic model particle velocities are assumed to be governed by a parametrized equicontinuous family of Ornstein-Uhlenbeck processes (OU-processes). Since the OU parameters are themselves functions of a more fundamental parameter, namely local particle concentration, the model operates with a nested parametrization scheme. Since local particle concentration is subject to change as the system evolves, the structure of the model is similar, in general, to that of random processes in random environments. In the special case considered here process parameters are functions of functionals over the state space of the system.

This complex structure is described in Section 2. The remainder of the paper then focuses on various aspects of the model. Section 3 presents a procedure for modelfitting and introduces satisfactory parameter estimators. Some of the suggested estimators are based, via a conditional maximum likelihood approach, on recent approximate solutions of first-passage time problems for integrated Ornstein-Uhlenbeck processes (Hesse (1990)).

Section 4 deals with computational aspects. The model easily lends itself to implementation and simulation. Incrementally, particles individually and simultaneously evaluate the system configuration (with respect to themselves) and determine updates of the fundamental parameter local particle concentration at their position. Then they perform velocity transitions governed by Ornstein-Uhlenbeck processes with these updated parameters. Assuming constant acceleration during the time increment this leads to a new state of the system after time Δt and, after local particle concentration has been updated again, to new parameters for the velocity processes. This scheme can easily be made into an algorithm for incremental system evolution and a detailed description is given in section 4.

The model has been implemented (by E. Ramos) on an Apollo Domain DN 600 with high resolution colour graphics driven by the software package PRIMH. However, it can also be implemented on other devices with graphics tools such as Suns, etc. The

implemented model constitutes an enormously powerful exploratory tool for hydrologists and rheologists.

Section 5 gives a brief discussion of directions for future research and of possible generalizations of the model.

We also mention that a motion picture has been produced using frame by frame photography on a computer simulated system with 1000 particles.

1. Previous Approaches to Sedimentation.

Since particle sedimentation is a physically well-defined phenomenon in the domain of continuum mechanics, the methods of fluid dynamics constitute legitimate tools to analyze the dynamics of systems in sedimentation. These methods proceed in principle, by setting up the equations of motion for all particles and all fluid flows generated by particle movement. Clearly, the dimensionality of this approach is much too high for the equations of motion to be solvable and for the problem to be tractable. However, since every model with claims to an accurate description of the phenomenon needs to be fluid-dynamically sound we will in this section briefly review the hydrodynamics of sedimentation.

1.1. *The Hydrodynamics of Sedimentation.*

Consider a particle system consisting of a finite number n of particles P_i, $i = 1, \ldots, n$, that are immersed in a viscuous fluid which is confined to some container D. Let S_i, S_D denote the surface of the i-th particle and the walls of the container D, respectively. Both S_i and S_D are subsets of $\mathbb{R}^3$, S_i depends on time t.

Fluid dynamics aims to determine the velocity field $V(x, t)$ for $x \in D$ and all $t \geq 0$. A more detailed account of what follows can be found in Happel and Brenner (1965).

Let Q_i be any fixed point in the interior of the i-th particle and denote by V_{tr}^i, V_r^i the instantaneous translational and rotational velocity of Q_i, respectively. Then, if e_i is the position vector of any point relative to an origin at Q_i, we obtain the following boundary conditions

$$V = V_{tr}^i + V_r^i \times e_i \quad \text{on each } S_i \tag{1.1}$$
$$V = 0 \quad \text{on } S_D$$

for the equation of motion

$$\lambda\left(\frac{\partial V}{\partial t} + V \cdot \nabla V\right) = -\nabla p + \eta \nabla^2 V + \lambda F, \tag{1.2}$$

where dependence on x and t has been suppressed to simplify notation. Here F is the external body force per unit mass. The other quantities are local fluid density λ, fluid viscosity η, and hydrostatic pressure p. For systems which settle under the influence of gravity only, F is equal to the local acceleration g.

Since we are using a linearized version of the equations of motion and due to the

linearity of the boundary conditions it is possible to decompose V into a translational component $\overline{V}$ satisfying only the V_{tr}^i part of Equation (1.1), and a rotational component ϖ satisfying the $V_r^i \times e_i$ part. Let $\overline{V}_i$ be the velocity field created when the i-th particle translates with instantaneous velocity V_{tr}^i, while all other particles are at rest. Similarly, let ϖ_i be the velocity field created when the i-th particle rotates with angular velocity V_r^i about an axis through Q_i while all other particles are at rest. The total velocity field is then the superposition of the fields $\overline{V}_i$ and ϖ_i. Hence

$$\overline{V} = \sum_i \overline{V}_i, \qquad \varpi = \sum_i \varpi_i, \qquad V = \overline{V} + \varpi.$$

Each $\overline{V}_i$, ϖ_i satisfies the boundary conditions

$$\overline{V}_i = V_{tr}^i \text{ on } S_i$$
$$\overline{V}_i = 0 \text{ on } S_j, \; j \neq i.$$

and

$$\varpi_i = V_r^i \times e_i \qquad \text{on } S_i$$
$$\varpi_i = 0 \qquad \text{on } S_j, \; j \neq i.$$

Now, if ${}_j\overline{F}_k$ is the hydrodynamic force exerted by the fluid on the k-th particle as a result of the translational motion $\overline{V}_j$ of the j-th particle, then

$${}_j\overline{F}_k = \int_{S_k} \Pi_j \cdot dS$$

where Π_j is the appropriate pressure tensor.

Similarly, the hydrodynamic torque about Q_k exerted by the fluid on the k-th particle due to translational motion of the j-th particle $\overline{V}_j$ is

$$ {}_j\bar{T}_k = \int_{S_k} e_k \times (\Pi_j \cdot dS). $$

Total force and total torque are equal to the sum of these contributions, i.e.

$$ \bar{F}_k = \sum_j {}_j\bar{F}_k, \quad \bar{T}_k = \sum_j {}_j\bar{T}_k. $$

All this is analogous for force ${}_j\bar{\bar{F}}_k$ and torque ${}_j\bar{\bar{T}}_k$ due to rotational movement of only the j-th particle and all other particles at rest:

$$ {}_j\bar{\bar{F}}_k = \int_{S_k} \bar{\Pi}_j \cdot dS $$

$$ {}_j\bar{\bar{T}}_k = \int_{S_k} e_k \times (\bar{\Pi}_j \cdot dS) $$

$$ \bar{\bar{F}}_k = \sum_j {}_j\bar{\bar{F}}_k $$

$$ \bar{\bar{T}}_k = \sum_j {}_j\bar{\bar{T}}_k. $$

It is well-known that both rotational and translational components of force and torque can be written in terms of translation and rotation tensors:

$$ \begin{aligned} {}_j\bar{F}_k &= -\eta\, \psi_{kj} \cdot \dot{V}^j_{tr} \\ {}_j\bar{T}_k &= -\eta\, \Psi_{kj} \cdot V^j_{tr} \\ {}_j\bar{F}_k &= -\eta\, \Theta_{kj} \cdot V^j_r \\ {}_j\bar{T}_k &= -\eta\, \Omega_{kj} \cdot V^j_r \end{aligned} \tag{1.3} $$

ψ_{kj}, Ψ_{kj}, Θ_{kj}, Ω_{kj} are second order tensors. These depend only on the size and shape of the particles, their initial configuration, the choice of coordinate system, and the Q_i. The tensors are, in particular, independent of the properties of the fluid.

Summing up these component forces and torques one finally arrives at the following coupled system of equations for total force F_k and total torque T_k:

$$F_k = -\eta \sum_{j=1}^{n} (\psi_{kj} \cdot V_{tr}^j + \Theta_{kj} \cdot V_r^j)$$

$$T_k = -\eta \sum_{j=1}^{n} (\Psi_{kj} \cdot V_{tr}^j + \Omega_{kj} \cdot V_r^j)$$

where the summation is on adjacent indices.

One may concisely express these relations as

$$\mathbf{F} = -\eta \mathbf{K} \cdot \mathbf{V} \tag{1.4}$$

where **F** is the so-called wrench matrix, **V** the screw velocity matrix, and **K** the grand-resistance matrix (see Happel and Brenner (1965) for definitions). For any multiparticle system, **K** is a positive definite and symmetric matrix and Equation (1.4) may, in principle, be solved by inverting this non-singular matrix **K**. However, except perhaps in dilute suspensions, determination of the grand-resistance matrix is difficult at best and even numerical attempts are unfruitful for moderate system size.

The above approach if tractable would reward us with complete trajectories for all particles and fluid flows. For practical purposes this degree of detailedness of information is usually not needed. Some workers (Kynch (1952), Fitch (1962)) have therefore developed approaches that are satisfied with making inferences about average particle behavior.

1.2. *Kynch's Theory of Sedimentation.*

Kynch (1952) operates with the two main assumptions that the settling velocity of a

particle depends only on local particle density ρ and that this density is constant over horizontal layers of the slurry. Together with the additional requirements that wall effects are negligible, that particles have equal size and shape, and that their velocity tends to zero as ρ increases towards its maximum these assumptions then make it possible to derive the time evolution of certain characteristics of the system from a continuity equation. We briefly demonstrate this.

Define the flux Γ as

$$\Gamma(x,t) = \rho(x,t) \cdot V(x,t)$$

where $x \in \mathbf{R}$ is the height above the bottom of the fluid. Γ can be interpreted as the number of particles crossing a horizontal cross-section per unit area and unit time. If Γ varies with x, then so does ρ.

Consider two layers at x and x + dx. Then the change in concentration in this slice is equal to the difference between the inflow of particles $\Gamma(x + dx, t)$ through the upper layer and the outflow $\Gamma(x, t)$ through the lower layer, per unit area:

$$\frac{\partial}{\partial t}(\rho(x,t)\,dx)dt = (\Gamma(x + dx, t) - \Gamma(x,t))dt.$$

This implies

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\partial \Gamma(x,t)}{\partial x}$$

which can be written as

$$\frac{\partial \rho(x,t)}{\partial t} + \psi(\rho(x,t)) \cdot \frac{\partial \rho(x,t)}{\partial x} = 0 \tag{1.5}$$

with

$$\psi(\rho) = -\frac{d\Gamma}{d\rho}.$$

Equation (1.5) is known as the continuity equation. It may be interpreted in the following way: If on a graph where position x is plotted against time t, curves are drawn through points that have the same concentration (isoconcentration curves) then the coordinates (x, t) and $(x + dx, t + dt)$ of two points on such a curve are related by

$$\rho(x + dx, t + dt) = \rho(x, t)$$

and hence

$$\frac{\partial \rho}{\partial x} dx + \frac{\partial \rho}{\partial t} dt = 0. \tag{1.6}$$

Combining (1.5) and (1.6) shows that the slope of such a curve is given by

$$\frac{dx}{dt} = \psi(\rho)$$

and since ρ is constant along the curve these curves must be straight lines. For every given point in the positive (x, t) quadrant below the top of the dispersion there is exactly one such line that goes through the point. Clearly, the starting point of these lines, $(x, t = 0)$, is determined by the initial concentration and in a region where this concentration is continuous no two lines intersect. See Kynch (1952) for a diagram.

Another way to view these simple results is in terms of propagation of concentration: A given value of the concentration is propagated through the dispersion with velocity $\psi(\rho) = -d\Gamma/d\rho$. Isoconcentration curves in x versus t diagrams and also Γ versus ρ

curves are characteristics of a particular dispersion. Kynch (1952) demonstrates how to make inferences about the system based on them.

The theory predicts the formation of a particle fluid interface and is also able to make statements about the variation of settling velocities over time. However, due to the restrictive nature of the model assumptions the detailedness and validity of these inferences is limited.

Most unsatisfying, of course, is the assumption that there is no velocity variation at given concentration. This is clearly false, and the stochastic model advanced in the following section eliminates this defect.

2. A Stochastic Model for Sedimentation.

The stochastic model of this section is the result of a compromise between an essentially intractable approach (hydrodynamics) and an approach that utilizes unrealistic and overly restrictive assumptions (Kynch's theory). It is a fruitful symbiosis between hydrodynamic and stochastic concepts: Individual particle trajectories are modelled according to fluid dynamic principles and system behavior is treated stochastically.

The basics of the model were introduced by Pickard and Tory in 1977. It has since then been refined and undergone revision (see Pickard and Tory (1979, 1982, 1986)) and some work has been done since then (see e.g. Hesse (1987)).

The model rests with its fundamentals on only three major pillars. These are

1. a family of stochastic processes governing particle velocity transitions
2. a functional parametrizing this family of stochastic processes
3. a concept (equicontinuity) providing the bridge between 1. and 2.

Although sedimentation is a phenomenon in three dimensions we will here for reasons of simplicity (but without loss of conceptual generality) reduce the space dimensions to two. Only vertical particle movement is considered, horizontal and rotational velocities are ignored.

To introduce some notation, let $D \subset \mathbb{R}^2$ be the container in which sedimentation takes place and let $X_i(t) \in D$ be the position of the (center of gravity of the) i-th particle at time t, $V_i(t)$ its (vertical) velocity at that time. Then

$$\{(X_i(t), V_i(t)),\ t \geq 0,\ i = 1, \ldots, n\}$$

describes the evolution of the sedimenting system over time. An alternative characterization is offered by

$$\{P(x,t),\ x \in D,\ t \geq 0\}$$

where

$$P: D \times \mathbb{R}^+ \rightarrow \{0,1\}$$

with

$$P(x,t) = \begin{cases} 1 \text{ if at time t a particle is positioned at } x \in D \\ 0 \text{ otherwise} \end{cases}.$$

We start with a discussion of the stochastic velocity processes.

2.1. *The Velocity Processes*

Consider a particle with position $X(t)$ at time t. At any given time it is subject to the following forces

a. gravitation F_g

b. friction F_f

c. Langevin force F_L

Gravitation $F_g = mg$ is proportional to the mass m of the particle. Friction $F_f = -\tau V(t)$ is taken to be proportional to particle velocity $V(t)$ but its direction is opposite to velocity (Stokes friction). The Langevin force is best thought of as being stochastic. It is due to the thermal movements of the fluid molecules and it exerts an increasing influence with decreasing particle mass. Sedimentation typically deals with particle sizes of orders of magnitude where this stochastic force cannot be ignored. It will be modelled as white noise, the formal derivative of Brownian motion $B(t)$.

Given the above forces, Newton's law then gives rise to the following stochastic differential equation:

$$mdV(t) = mgdt - \tau V(t)dt + dB(t)$$

the solution of which is given by an Ornstein-Uhlenbeck process with drift μ, friction parameter β and variance σ^2. The parameters μ, β, σ^2 depend on characteristics of the

system such as m, τ, etc.

A parametrized family of Ornstein-Uhlenbeck processes is therefore a reasonable choice of processes to govern incremental particle velocity transitions.

We now discuss the nested parametrization of these processes.

2.2. *Parametrization*

It is a key hydrodynamic fact that identical particles in the same "environment" exhibit the same settling behavior. "Environment" is here interpreted in a very broad sense and includes, in particular, positions of other particles, fluid flows and possibly internal pressures and gravitational and external forces.

If a particle has complete "knowledge" of its environment it invokes the laws of physics and "computes" its incremental trajectory in a deterministic fashion. But obviously, for the purpose of any modelling with relevance in applications, environment in the above sense is a much too high dimensional parameter. An attempt is therefore made to summarize environment by a one-dimensional parameter which tries to capture the main determinants of incremental particle behavior. The remaining factors are combined to velocity variation (via stochastic processes) at the given value of the summary parameter.

Heuristically, a particle being equipped with only a partial knowledge of its full environment (in the form of the current value of the summary parameter) selects its

incremental velocity transition from a distribution parametrized by a function of this summary parameter.

The stochastic model operates with local particle concentration as the major determinant of incremental particle behavior. This choice is physically motivated and has been confirmed experimentally.

Local particle concentration is most easily defined via $\{P(x,t),\ x \in D,\ t \geq 0\}$ which characterizes system configuration and its evolution.

Definition: (Local particle concentration $c(x,t)$)

Local particle concentration is a kernel-smoothed version of relative configuration, i.e.

$$c(x,t): D \times \mathbb{R}^+ \rightarrow (0,1)$$
$$c(x,t) = \iint_D K(x-y)\,P(y,t)\,dy$$

for some kernel $K: \mathbb{R}^2 \rightarrow \mathbb{R}^+$ that integrates to one and is typically taken to be unimodal and sometimes taken to vanish outside of a neighborhood of the origin.

Many different kernel functions will presumably lead to qualitatively similar system behavior. The actually utilized kernel function was chosen on the basis of considerations of computational efficiency. We address computational aspects in a more detailed fashion in section 4.

Local particle concentration is a functional whose major purpose is the parametrization of the distributions that govern incremental velocity transitions over a time interval Δt. These distributions are derived from a family of Ornstein-Uhlenbeck processes which are parametrized as usual by drift μ, friction coefficient β, and variance σ^2. This reveals that the stochastic model in fact employs a nested two-stage parametrization scheme: The Ornstein-Uhlenbeck parameters are themselves functions of the more fundamental parameter c which evolves over time. It is clear that these parameter functions cannot be obtained theoretically but can only be determined experimentally from actual systems in sedimentation. We address issues of parameter estimation and modelfitting in section 3.

The above principles also give a great deal of insight into the evolution of the entire system during sedimentation: At time t, each particle individually and all particles simultaneously determine their specific local particle concentration $c(X_i(t), t)$. In the family of Ornstein-Uhlenbeck processes particles then adjust the parameters to the updated values $\mu(c(X_i(t), t))$, $\beta(c(X_i(t), t))$ and $\sigma^2(c(X_i(t), t))$ and sample their velocity transitions from the corresponding conditional distributions (i.e. given $V_i(t)$). In this fashion one obtains $V_i(t + \Delta t)$, for $i = 1, \ldots, n$. To compute particle positions at time $t + \Delta t$ an assumption is necessary for $V_i(t + \delta t)$ for $\delta t \in (0, \Delta t)$. It makes both physical and analytic sense to assume constant acceleration during $[t, t + \Delta t]$. Particle

positions $X_i(t + \Delta t)$ can then be computed and, again, $c(X_i(t + \Delta t), t + \Delta t))$ is available so that parameters can be updated to $\mu(c(X_i(t + \Delta t), t + \Delta t))$ etc.

2.3. *Equicontinuity*

From the above discussion it is clear that a concept is necessary which provides a link between the family of discrete Ornstein-Uhlenbeck processes and their parametrization. The stochastic model employs the concept of equicontinuity. If, at local particle concentration c, $f_c(v, t, u)$ denotes the probability density that a particle with velocity u will have velocity v after time t, then the following assumption is made about the family of densities $\{f_c, c \in (0, 1)\}$:

Assumption: For every $c \in (0,1)$ and every $\varepsilon > 0$ there exists a $\delta = \delta(c, \varepsilon)$ such that for all u, v and $t \geq T_0$, for some $T_0 > 0$

$$c' \in (0, t), \ |c - c'| < \delta(c, \varepsilon) \Rightarrow |f_c(v, t, u) - f_{c'}(v, t, u)| < \varepsilon.$$

Hence $\{f_c, c \in (0,1)\}$ is an equicontinuous family on $V \times V$, say, the cross product of the set of attainable velocities.

One might wonder why uniformity is required for all t larger than some T_0 only. The reason is that as $t \to 0$, f_c approaches a delta function and the above condition with $t \geq T_0$ replaced by $t \geq 0$ would be much too restrictive. However, as stated, the equicontinuity requirement seems mild. It can be justified heuristically: Since local particle concentration is the major singlemost factor governing particle behavior, small

changes in concentration should only cause small perturbations of the velocity transition structure of particles.

The concept of equicontinuity, together with the parametrization by local particle concentration and the fact that velocity transitions are governed by a family of discrete Ornstein-Uhlenbeck processes has far-reaching implications. These implications, as we will see, make efficient simulation of the stochastic model possible. We list some important implications in a loose fashion. The proofs are simple and are left to the reader.

Implication 1: For all $c \in (0, 1)$ and all $u \in V$, the probability densities $f_c(v, t, u)$ converge to a steady-state density as $t \to \infty$: i.e. $\lim_{t\to\infty} f_c(v, t, u) = g_c(v)$, say.

Implication 2: The steady state densities g_c are continuous functions of c.

Implication 3: The Ornstein-Uhlenbeck parameters $\mu(c)$, $\beta(c)$, $\sigma^2(c)$ are continuous functions of c.

Implication 4: If local particle concentration changes sufficiently little along the trajectory of a particle during a time interval $[t_1, t_2]$ then this particle can be treated as remaining under the influence of a single Ornstein-Uhlenbeck process (as a uniform approximation) during

$[t_1, t_2]$.

Implication 5: If in a region $D_0 \subset D$ local particle concentration changes sufficiently little then this region can be characterized by a single Ornstein-Uhlenbeck process (as a uniform approximation).

Implication 6: Every sedimenting system can be characterized by finitely many Ornstein-Uhlenbeck processes (as a uniform approximation).

It should be pointed out that the stochastic model of sedimentation is not a steady-state model. Although, at any given time, the conditional velocity processes are converging to steady-state this state might not be reached if significant concentration changes occur along particle trajectories before the Ornstein-Uhlenbeck velocity processes can converge.

In the next section we will address the problem of estimating the parameter functions $\mu(c)$, $\beta(c)$ and $\sigma(c)$ from actual systems in sedimentation.

3. Modelfitting and Parameter Estimation.

In the context of the stochastic approach, modelfitting amounts to determination of the parameter functions $\mu(c)$, $\beta(c)$ and $\sigma^2(c)$ from a physical system in sedimentation. Some experimental work has been done to study the effects of different concentrations on the velocity distribution of sedimentating particles, see e.g. Shannon et. al. (1964),

Johne (1965), Koglin (1971). Shannon et. al. (1964) study, among other things, the steady-state mean velocity of particles as a function of global (rather than local) particle concentration γ (the total proportion of solids). Their results contradict earlier beliefs that average steady-state velocity decreases monotone with increasing global concentration γ. To the contrary, there is an interval where the mean velocity vs. concentration curve has positive slope and a maximum at some $\gamma_0 \neq 0$.

The reason for this behavior is the formation of particle clusters and the fact that these clusters tend to settle faster than individual particles. In very dilute suspensions particles are so far apart that hardly any interactions occur and faster settling clusters are virtually non-existent. When concentration is increased towards γ_0, the tendency for cluster formation also increases and their presence increases average settling velocity. When concentration is increased further (beyond γ_0) the number and size of clusters increases also. Eventually cluster frequency becomes so high, that clusters slow each other down, hence decreasing average velocity again. It can be expected that the dependence of Ornstein-Uhlenbeck drift velocity $\mu(c)$ on local particle concentration is qualitatively quite similar.

As to β and σ^2, their dependence on concentration (both local and global) does not seem to have been investigated at all. We propose, in this section, several estimators that allow to make use of extensive industrial data bases containing, for varies concen-

trations, particle sizes and shapes, mostly transit time data. For particles starting at $t = 0$ with velocity $V(0)$ it is measured how long it takes them to first cross several boundaries at distances $x, 2x, 3x, \ldots$. The estimation procedure will be demonstrated on some experimental data. These data were obtained at the Universität Karlsruhe (FRG) by T. Lasar. We would like to thank B. Koglin for making them available to us. A small subset of the dataset (for global concentration $\gamma = 0.0023$) is given in the appendix.

Parameter estimation based on transit times leads to the first-passage problem for an integrated Ornstein-Uhlenbeck process with parameters $\mu(c(\cdot,\cdot))$, $\beta(c(\cdot,\cdot))$, $\sigma^2(c(\cdot,\cdot))$. For the purpose of estimating these parameter functions one will have to ensure, through the choice of x, that along the particles trajectories (until boundary crossing) local concentration is essentially constant and equal to c, say. Then

$$X_i(t) = X_i(0) + \int_0^t V_i(s)\,ds$$

where $V_i(s)$ is an Ornstein-Uhlenbeck process with parameters $\mu(c)$, $\beta(c)$, $\sigma^2(c)$. Define

$$\tau(x) = \min\{t \geq 0 : X_i(t) = x \mid X_i(0) = 0,\ V_i(0) = v + \mu\}.$$

Hesse (1990) derives several accurate global approximations for the density $g(t)$ of $\tau(x)$, in particular, as the boundary becomes increasingly remote

$$g_1(t) = x\beta(2\pi\sigma^2 t^3)^{-1/2}\exp(-\beta^2(x - \mu t)^2/(2\sigma^2 t)) \tag{3.1}$$

with

(3.2) $$\text{mean} = x\mu^{-1}$$

(3.3) $$\text{variance} = \sigma^2 x\mu^{-3}\beta^{-2}.$$

Another approximation (accurate if $(3x - vt)/2t$ is large and β is small) is given by

(3.4) $$g_2(t) = \left(\frac{3x - (v+\mu)t}{2t} - \frac{\beta}{8}(3(x - \mu t) - vt)\right)\phi(x)$$

where $\phi(x)$ is the density of the normal distribution with mean $= (v/\beta)(1 - e^{-\beta t}) + \mu t$ and variance $= (\sigma^2/2\beta^3)(2\beta t + 4e^{-\beta t} - e^{-2\beta t} - 3)$.

Finally, and globally more accurate than $g_2(t)$ in (3.4),

(3.5) $$g_3(t) = g_2(t)(\Phi(\lambda(t)) + (\lambda(t))^{-1}\psi(\lambda(t)))$$

where ψ and Φ are the standard normal density and distribution functions, respectively, and

$$\lambda(t) = (3x - (v+\mu)t - (\beta t/4)(3(x - \mu t) - vt))/(\sigma t^{3/2} - \sigma\beta t^{5/2}/8).$$

Based on these approximations conditional maximum likelihood estimators may be derived, see Hesse (1990) for details. Briefly, the random variable

$$Y = \exp(\tau(x) + (\tau(x))^{-1})$$

is approximately of algebraic tail-type in the sense that

$$P(Y \geq y) \approx \text{const.}\, y^{-\alpha}$$

with $\alpha = 2\beta^2\sigma^{-2}x\mu\pi^{-1}$ and $y \geq B$ for some B.

Hence, if k is appropriately chosen

(3.6) $$W(i) = i\ln(Y_{(i)}/Y_{(i+1)}) \qquad i = 1, \ldots, k$$

are independent, identically distributed exponential random variables with parameter α.

Here

$$Y_{(1)} \geq Y_{(2)} \geq \cdots \geq Y_{(n)}$$

are the order statistics in descending order. The number $k + 1$ of extreme order statistics to be used in (3.6) can be determined by simple data analytic methods. Since x is known and μ can usually be estimated using different methods the above strategy gives access to $\sigma^2\beta^{-2}$ but not to σ^2 and β^2 separately.

Similarly, one may also make inferences based on the left hand tail of the distribution of $\tau(x)$. Define

$$Z = \exp((x - \mu\tau(x))^2 (\tau(x))^{-3})$$

which is also of algebraic tail type, namely

$$P(Z > z) \approx \text{const.}\, z^{-\frac{3\pi}{2\sigma^2}} \tag{3.7}$$

for z large. Hence the above methods may be used to estimate σ^2.

Since this approach makes use of only a fraction of the data set it is clear that it requires relatively large data sets to produce estimates with acceptable standard deviation.

We give another strategy to estimate β based on the following argument:

Since

$$X(t) = \int_0^t V(s)\, ds$$

then for any fixed T

$$\mathrm{Cov}\,(X(T), X(nT) - X((n-1)T) = \int_0^T \int_{(n-1)T}^{nT} E(V(t_1)\,V(t_2))\,dt_2\,dt_1$$

$$= \frac{\sigma^2}{2\beta} \int_0^T \int_{(n-1)T}^{nT} (e^{2\beta t_1} - 1)\,e^{-\beta(t_1+t_2)}\,dt_2\,dt_1$$

$$= \frac{\sigma^2}{2\beta^3} (1 - e^{-\beta T})^3\,e^{-(n-2)\beta T}.$$

Hence

$$(3.8) \qquad \frac{\mathrm{Cov}\,(X(T)/T, (X(nT) - X((n-1)T))/T)}{\mathrm{Cov}\,(X(T)/T, (X(2T) - X(T))/T)} = e^{-(n-2)\beta T}.$$

Note that $(X(nT) - X((n-1)T)T^{-1}$ is the average velocity during the interval $[(n-1)T, nT]$. The relation in (3.8) will be approximately true (with T on the right hand side of (3.8)) replaced by $E(\tau(x)))$ for average velocities over space intervals, i.e. for $X(\tau(nx) - \tau((n-1)x))^{-1}$ computed from first passage times.

We therefore estimate β as the slope of the linear regression through the origin of

$$(3.9) \qquad \log\left[\frac{\mathrm{Cov}\,((\tau(x) - \tau(0))^{-1}, \tau(2x) - \tau(x))^{-1}}{\mathrm{Cov}\,((\tau(x) - \tau(0)), \tau(nx) - \tau((n-1)x))^{-1}}\right] \quad \text{on} \quad (n-2)x\mu^{-1}.$$

We demonstrate the estimation of parameters with the data set given in the appendix.

The assumption will be made that over the distances considered (up to the boundary at 800mm) the suspension remains uniformly mixed in the large. This implies that for any of the 30 particles on which measurements were obtained local particle concentration remains essentially constant along their trajectories. Hence the particles remain under the influence of a single Ornstein-Uhlenbeck process and the parameters are

constants: $\mu(c)$, $\beta(c)$, $\sigma^2(c)$ with $c = 0.0023$.

It is also assumed that the velocity distribution with which particles cross the first boundary is the steady-state boundary crossing velocity distribution and that the runs of the $n = 30$ particles are independent.

As can be seen, transit times for different settling intervals are highly correlated indicating that on each subinterval of length 100mm approximation of the displacement process $X(t)$ by a Brownian motion is not valid. Hence $g_1(t)$ is presumably not a satisfactory approximation to the first passage time density on each subinterval. This is consistent with rough estimates (based on physical considerations) of the magnitude of β. They indicate that, on the average, $\beta(\tau(nx) - \tau((n-1)x))$ will not be large, but $\beta(\tau(8x) - \tau(0))$ will be. Thus $g_1(t)$ approximates the first-passage density well over the entire settling distance of 800mm.

This last assumption gives access to μ and σ^2/β^2 via the method of moments or maximum likelihood applied to observed transit times over the entire distance of 800mm. But it does not give access to σ^2 and β^2 separately. To disentangle these the methods based on (3.9) or, for larger data sets, (3.7) may be used. For the data set in the appendix we obtained the following estimators ($\tau_i(x)$ denotes the observed transit time of the i-th particle to the boundary at x):

- $\hat{\mu}$ is the estimator of μ computed as the sample mean of $8x/(\tau(8x) - \tau(0))$ where $x = 100mm$

- $(\sigma^2\beta^{-2})\hat{}$ is the maximum likelihood estimator based on the approximation $g_1(t)$ i.e.

$$(\sigma^2\beta^{-2})\hat{} = \frac{1}{n}\sum_{i=1}^{n}(8x - \mu(\tau(8x) - \tau(0)))^2/(\tau(8x) - \tau(0))$$

- $(\sigma^2\beta^{-2})\tilde{}$ is the method of moments estimator based on $\mathrm{var}(X(T)/T) \approx \sigma^2\beta^{-2}T^{-1}$ for large T. For large x, the variance of $8x/(\tau(8x) - \tau(0))$ satisfies approximately the same relation (with T replaced by $8x\hat{\mu}^{-1}$).

- $\hat{\beta}$ is the estimator of β obtained from (3.9).

For the data set given in the appendix:

$\hat{\mu} = 2.113$ with SE $= 0.05$, $(\sigma^2\beta^{-2})\hat{} = 29.8$, $(\sigma^2\beta^{-2})\tilde{} = 30.4$, $\hat{\beta} = 0.007$ (with SE $= 0.0005$)

4. Computational Issues.

Although conceptually the model is simple, its structure is complex and it is apriori not obvious whether it lends itself to efficient implementation and simulation. The bottle-neck is the simultaneous updating of parameters, velocities, and positions. The updating of local particle concentration $c(x,t)$ is especially troublesome. It is possible however to introduce several simplifying features into the model structure without essentially changing the qualitative behavior of evolving particle systems. These

simplifications, discussed in the sequel, greatly enhance computational efficiency.

1. A standardized, dimensionless version of the model can be obtained which also reduces the number of parameter functions to only one. This is achieved by measuring particle velocity in multiples of drift velocity μ and time in multiples of βt, i.e.

$$t' = \beta t, \quad v' = v\mu^{-1} \text{ and hence } x' = \beta\mu^{-1} x.$$

In this new coordinate system $\mu' = \beta' = 1$ and $\sigma' = \sigma\mu^{-1}\beta^{-1/2}$ is the only remaining relevant parameter.

2. The original definition of local particle concentration $c(x,t)$ can be replaced by a lower-dimensional and computationally more efficient version. To obtain this define for $y \in \mathbb{R}$

$$Q(y,t) = \iint_{D \cap [y, y+\Delta y] \times \mathbb{R}} P(x,t)\,dx$$

which is the proportion of the horizontal layer at y that is occupied by particles. The definition of local particle concentration is then revised to

$$c^*: \mathbb{R} \times \mathbb{R}^+ \rightarrow [0,1]$$
$$c^*(y,t) = \int_{D^*} K^*(y - y')\,dQ(y',t)$$

where

$$D^* = \{y \in \mathbb{R}: (z,y) \in D \text{ for some } z \in \mathbb{R}\}$$

and $K^*: \mathbb{R} \rightarrow \mathbb{R}$ is a one-dimensional kernel. In this interpretation, c^* is a sim-

ple convolution of Q with K^*. Consequently, c^* may be efficiently updated simultaneously for all layers by the Fast Fourier Transform algorithm. If, in addition, Gaussian kernels are used, then this further increases computational efficiency. By changing the bandwidth of these kernel smoothers, systems that exhibit very different qualitative behavior during their evolution may result. Note that the assumption of constant concentration across horizontal layers was also made by Kynch (1952).

3. When simulating the evolution of the particle system both space and time need to be discretized. We chose the increment Δy in such a way that the height of the sedimentation vessel was divided into about 100 horizontal layers. The time scale was discretized to $k\Delta t$, $k = 0,1,2,...$ with a choice of Δt so that on the order of 1000 steps were necessary for most particles to reach the bottom of the vessel.

   One may also discretize the concentration interval c (or c^*) to $c_m = m\Delta c$, $m = 0, 1, \ldots, [(\Delta c)^{-1}]$ where $[x]$ is the integer part of x. The i-th particle will then remain under the influence of the Ornstein-Uhlenbeck process with parameters $\mu(c_{m_0})$, $\beta(c_{m_0})$, $\sigma^2(c_{m_0})$ during the time interval $[k_1 \Delta t, k_2 \Delta t]$ if

$$|c(X_i(k\Delta t), k\Delta t) - c_{m_0}| \leq |c(X_i(k\Delta t), k\Delta t) - c_m|$$

   for all $k = k_1, k_1 + 1, \ldots, k_2$ and all m. Similarly for the lower-dimensional version c^*.

4. The discretization of time makes an assumption necessary that specifies the behavior of particles during the intervals $(k\Delta t, (k+1)\Delta t)$ for each $k = 0, 1, 2, \ldots$. As indicated in section 2, the model assumes constant acceleration during these intervals. This amounts to approximation of the integral in

$$X_i(t+\Delta t) = X_i(t) + \int_t^{t+\Delta t} V_i(t)\,dt,$$

by the trapezoidal rule of quadrature and leads to position being a quadratic spline. Hence, this assumption also implies the use of a quadratic interpolation scheme when determining boundary crossing times, as needed for purposes of parameter estimation.

5. During simulation the number of visually displayed particles was limited to about 1000. This is a necessary compromise between realism and computational tractability.

6. Although sedimentation is a phenomenon in three dimensions, vertical motion is the most important. However, to make the evolution of the particle system more realistic one may model horizontal motion by superimposing zero-mean Ornstein-Uhlenbeck processes. In addition, one may allow particle trajectories to overlap in order to indicate a third dimension.

5. Discussion.

The local structure of the stochastic model for sedimentation is very flexible and leaves considerable freedom for fine-tuning into particular applications. This flexibility includes the choice of stochastic processes (Ornstein-Uhlenbeck, Brownian motion, Bessel processes, others), the degree of refinement of the discretization of space and time, the choice of the kernel-smoother and hence the exact definition of local particle concentration, and the shape of the parameter functions $\mu(c)$, $\sigma^2(c)$ and $\beta(c)$ (or $\sigma'^2(c)$ in the dimensionless version).

This flexibility makes it possible to design models which exhibit widely different qualitative behavior such as the formation of dense particle layers, systematic or chaotic velocity variation, the formation of sharp or depleted interfaces, and many others. But the use and applicability of these models is not limited to particle sedimentation in fluids. Models of this type may also prove useful in describing the dynamics in chemical reactions, traffic flow patterns, etc.

The purpose of the stochastic model and especially its computer implementation is to equip engineers with an exploratory tool for their study of sedimentation phenomena. As described in this paper it covers the basic case of identical particles settling in a viscuous fluid under the influence of gravity only (i.e. no other external forces or internal pressures).

In the future it is hoped to incorporate such features as different particle species, non-spherical shapes and external forces, e.g. centrifugal forces, and laminar or even turbulent motion of the fluid medium. The study of slurries containing different particle species is of particular interest in applications. Problems of particle classification and particle separation into size fractions are industrially relevant.

The author became involved in this project when he joined the Department of Statistics at Harvard University in 1984 to work with D. Pickard. Some computational work was done at Queen's University in Kingston, Ontario, Canada and at the University of California at Berkeley. This work is dedicated to the memory of David Pickard.

Appendix.

The dataset for which we demonstrate the estimation of Ornstein - Uhlenbeck parameters in section 3 was obtained by T. Lasar at the Institut für Mechanische Verfahrenstechnik, Universität Karlsruhe. We would like to thank T. Lasar and B. Koglin for making these data available.

$\tau(x)-\tau(0)$	$\tau(2x)-\tau(x)$	$\tau(3x)-\tau(2x)$	$\tau(4x)-\tau(3x)$	$\tau(5x)-\tau(4x)$	$\tau(6x)-\tau(5x)$	$\tau(7x)-\tau(6x)$	$\tau(8x)-\tau($
46.3	50.9	46.1	36.8	41.6	41.0	38.3	41.6
57.4	50.7	53.6	46.5	36.4	32.2	24.8	26.2
66.5	47.5	46.8	51.0	56.6	56.9	48.1	48.6
49.8	41.8	42.8	49.7	40.7	42.2	45.6	44.3
65.1	71.9	60.7	50.5	47.9	62.1	66.0	68.2
55.6	42.8	39.3	36.2	41.6	52.0	48.1	53.4
51.1	63.3	49.9	36.1	40.6	36.7	47.8	55.9
48.1	49.9	49.5	45.8	56.7	75.2	65.1	63.8
44.5	49.0	58.4	43.7	46.5	52.4	52.2	52.6
45.8	43.2	41.8	39.7	30.7	32.4	34.0	36.2
62.6	50.3	51.9	52.3	56.7	50.6	65.2	63.8
60.5	55.1	56.9	57.9	55.0	57.4	64.7	54.1
55.1	52.7	50.9	44.4	42.2	37.2	48.6	41.9
33.8	38.6	45.3	34.6	34.6	37.7	43.9	40.8
56.8	55.1	48.1	41.9	52.1	44.4	38.3	38.8
65.8	57.4	52.9	42.6	50.4	54.3	58.2	58.0
64.6	60.0	52.7	50.8	52.9	44.9	38.1	39.8
40.3	42.5	47.4	49.2	46.4	38.4	35.1	39.9
35.3	37.9	39.4	37.3	41.1	39.4	41.2	37.5
54.3	51.8	43.0	50.2	64.8	65.2	59.2	55.9
37.5	35.8	39.5	57.4	69.5	65.9	58.2	49.1
50.3	45.8	33.3	33.6	41.1	54.0	53.5	40.3
51.0	44.1	38.1	40.6	41.9	35.8	41.7	47.7
60.4	41.8	39.9	34.6	37.9	43.8	40.6	42.5
75.4	65.3	57.8	55.2	50.5	45.7	43.3	36.0
43.6	37.3	39.1	40.3	41.3	35.4	37.9	52.8
47.4	51.4	53.9	60.6	53.9	52.0	45.2	42.6
58.0	54.5	47.3	38.4	45.9	45.5	50.3	51.7
49.2	64.1	64.9	59.9	60.7	55.8	45.7	47.3
58.9	55.5	48.4	41.8	44.3	37.2	34.0	39.2

Table 1: Observed transit-time data for 8 consecutive intervals of 100mm length (Limestone particles in silicone oil).

The experiments were conducted in a cylindrical sedimentation vessel of 114mm diameter with a monodisperse suspension of cylindrical limestone particles in silicon oil AK1000. Reynolds numbers were less than 0.006. Marked boundaries were placed 100mm apart (x = 100mm) starting about 200mm below the surface of the fluid. The first boundary also defines the zero of the vertical scale. Transit times for settling between boundaries were visually registered for 8 consecutive intervals. These are denoted by $\tau(nx) - \tau((n-1)x)$ for $n = 1, \ldots, 8$. $\tau(x)$ denotes the time until first crossing of the boundary at x. The suspension was initially uniformly mixed (with overall concentration c = 0.0023). Particles (n = 30 all together) for which passage times are obtained were first wetted with the liquid and then introduced at the axis of the sedimentation vessel below the fluid surface about 50mm above the first boundary at 0. The table contains values of $\tau(nx) - \tau((n-1)x)$ for $n = 1, \ldots, 8$.

References

1. Batchelor, G.K. Sedimentation in a dilute dispersion of spheres. *J. Fluid Mech.* **52**, 245-268 (1972)

2. Fitch, B. Sedimentation process fundamentals. *Trans. AIME* **223**, 129-137 (1962).

3. Happel, J. and Brenner, H. *Low Reynolds Number Hydrodynamics*. Prentice-Hall, Englewood Cliffs, N.J. (1965).

4. Hesse, C.H. The one-sided barrier-problem for an integrated Ornstein-Uhlenbeck process. Technical Report #250. Department of Statistics, University of California, Berkeley, CA 94720 (1990).

5. Hesse, C.H. Modelling sedimentation. Technical Report #125, Department of Statistics, University of California, Berkeley, CA 94720 (1987).

6. Johne, R. Einfluss der Konzentration einer monodispersen Suspension auf die Geschwindigkeit iher Teilchen. Dissertation Universität Karlsruhe (1965).

7. Koglin, B. Untersuchungen zur Sedimentationsgeschwindigkeit in niedrig konzentrierten Suspensionen. Dissertation Universität Karlsruhe (1971).

8. Kynch, G.J. A theory of sedimentation. *Trans. Faraday Soc.* **48**, 166-176 (1952).

9. Oliver, D.R. The sedimentation of suspensions of closely-sized spherical particles. Chem. Eng. Sci., 230-242 (1961).

10. Pickard, D.K. and Tory, E.M. A Markov model for sedimentation. *J. Math. Anal. Appl.* **60**, 349-369 (1977).

11. Pickard, D.K. and Tory, E.M. Experimental implications of a Markov model for sedimentation. *J. Math. Anal. Appl.* **72**, 150-176 (1979).

12. Pickard, D.K. and Tory, E.M. Extensions of a Markov model for sedimentation. *J. Math. Anal. Appl.* **86**, 442-470 (1982).

13. Pickard, D.K. and Tory, E.M. A Markov model for sedimentation: Fundamental issues and insights. Technical Report, Department of Mathematics and Statistics, Queens University, Kingston (1986).

14. Shannon, P.T., DeHass, R.D., Stroupe, E.P. and Tory, E.M. Batch and continuous thickening: prediction of batch settling behavior from initial rate data with results for rigid spheres. *Ind. Eng. Chem. Fundam.* **3**, 250-260 (1964).

15. Slack, G.W. and Matthews, H.W. The mutual interaction between sedimenting

particles, 1: The sedimentation of compact clusters of spheres in a viscous medium. Technical Paper No. 797, Chemical Defense Experimental Establishment, Porton (1961).

16. Richardson, J.I. and Zaki, W.N. Sedimentation and fluidization. *Trans. Inst. Chem. Engrs.* **32**, 35-53 (1954).