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Stochastic simulation of sedimentation

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Abstract

The slow sedimentation of small particles in a viscous fluid is a long-standing problem with many important applications. One-dimensional sedimentation of a suspension of rigid spheres in a Newtonian fluid involves three parameters: the mean, variance, and autocorrelation of the vertical component of particle velocities. The mean corresponds to Kynch's unique (or characteristic) velocity, the variance reflects the spatial and temporal variability of particle velocities, and the autocorrelation preserves the continuity of the velocity of each individual particle. To account for these properties, Tory and Pickard formulated a three-parameter Markov model in which identical particles in the same environment are governed, independently, by the same stochastic process. This model preserves the short-term predictability of deterministic solutions, but reflects the fact that detailed results from one experiment or computation provide only statistical predictions about results from others. Since the mean velocity determines many features of sedimentation, the Markov model essentially subsumes Kynch's theory as a special case. The model predicts that the distribution of particle velocities evolves toward a steady state. The hydrodynamic diffusion model for sedimentation was developed a decade later, but the solution of the resulting parabolic differential equation does not preserve the continuity of velocity. The Markov model, which does, thereby makes full use of experimental measurements of individual trajectories. We use it to simulate the sedimentation of very dilute suspensions of identical spheres. The three parameters are usually assumed to be functions of a concentration parameter that is a convolution of local concentrations with a Gaussian kernel, but a simpler approximation suffices for these suspensions. The simulation employs a fourth-order stochastic Runge-Kutta method developed by Honeycutt and adapted by Tory et al. The simulated results accurately reproduce observed phenomena and are amazingly realistic in appearance.

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1 Introduction

The success of Kynch's theory [1] reinforced the prevailing view that identical particles settled with the same velocity. However, experimental observations (summarized by Tory et al. [2] and Tory and Hesse [3]) established the spatial and temporal variability and the autocorrelation of particle velocities. On the basis of this work, Pickard and Tory formulated a three-parameter Markov model [4–7]. This stochastic model, which captures the principal features of sedimentation, assumes that identical particles in the same environment are governed, independently, by the same stochastic process [5]. Tory et al. [2] subsequently established the theoretical basis for this assumption. The model preserves the short-term predictability of deterministic solutions, but reflects the fact that detailed results from one experiment or computation provide only statistical predictions about results from others [2]. The Markov property is consistent with the dependence of Stokes solutions on current conditions only. Since the mean velocity determines many features of sedimentation, the Markov model essentially subsumes Kynch's theory as a special case. The model predicts that the distribution of particle velocities evolves toward a steady state.

2 A three-parameter Markov model

The three-parameter Markov model for sedimentation is the system of Ito stochastic differential equations for (vertical) position $X_k(t)$ and velocity $V_k(t)$ for $k = 1, \dots, N$ where N is the number of particles. If the solids concentration, φ, is constant in a large region, then

$$dX_k(t) = V_k(t)dt, \tag{1}$$

$$dV_k(t) = -\beta(\varphi)[V_k(t) - \mu(\varphi)]dt + \sigma(\varphi)\, dW_k(t), \tag{2}$$

where σ controls the variation of velocity increments, $-\beta(V-\mu)dt$ describes the strength with which individual velocities are shifted toward the steady-state ensemble value μ, and $W_k(t)$ denotes a Wiener process [5,8].

The most important parameter is the mean velocity, $\mu(\varphi)$, which was usually determined from the rate of fall of the interface. This works well for fairly concentrated suspensions, but not for very dilute suspensions in which the mean velocity exceeds that of the interface [2]. In dilute suspensions, μ must be determined from measurements of the velocities of individual particles. It is more informative to plot the solids flux, $f(\varphi) = \varphi\mu(\varphi)$, against φ. According to Kynch's theory [1,9], this flux plot completely determines the settling curve (height vs. time). Figure 1 shows the variation of solids flux with concentration for the system studied by Pickard and Tory [4]. The curve is a cubic spline clamped at $\varphi = 0$ and at $\varphi = 0.04$. For their system, the velocity of a single sphere settling in a cylindrical tank [10] yields $f'(0) = -4.73$ and matching Verhoeven's data [11] for more concentrated

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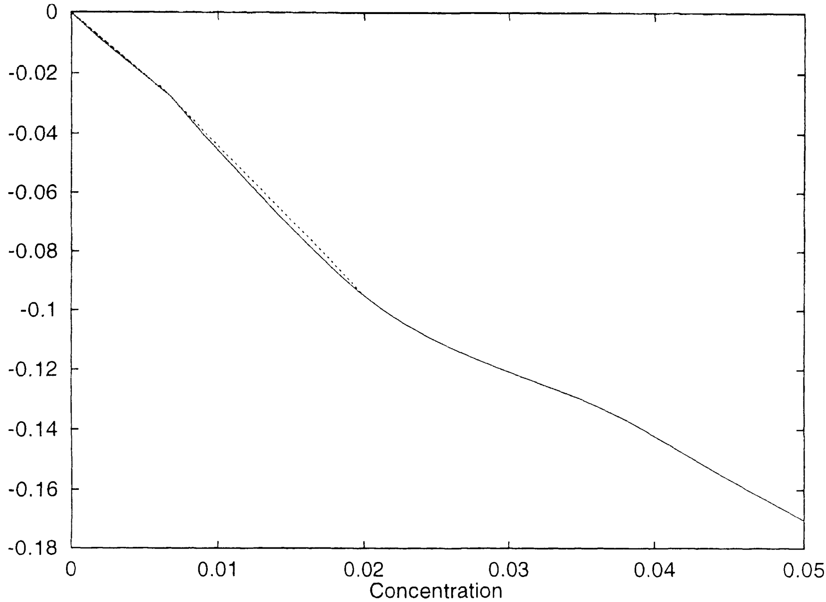

Figure 1: Flux plot for a very dilute dispersion of identical spheres. The chords indicate the discontinuities predicted by Kynch's theory.

suspensions requires that

$$f(\varphi) = -4.19\varphi(1-\varphi)^{4.032}, \quad 0.04 \leq \varphi \leq 0.05. \tag{3}$$

This is based on a Richardson-Zaki equation [12] that fits his interface data for a wide range of concentrations. Since the mean velocity in the bulk of the suspension that is still at the initial concentration cannot be greater (algebraically) than that of the interface, we have also used eqn (3) as an upper bound for the value of the flux at lower concentrations.

It is convenient to use the variance, σ_v^2, of the steady-state instantaneous velocity of the particles as one of the parameters. This is related to the parameter σ in eqn (2) by

$$\sigma^2 = 2\beta\sigma_v^2. \tag{4}$$

However, the steady-state value of the variance in suspensions that were uniformly mixed initially is very controversial [2,3,13]. We have used the dependence found by Segre et al. [13], but slightly increased the value of the constant in their eqn (3) to make the result agree with the experimental value for $\varphi = 0.02$. Also, we have combined that equation with the theoretical result for very dilute suspensions. The result,

$$\sigma_v = \begin{cases} 24.64\varphi^{1/2}, & 0 < \varphi < 0.003375, \\ -2.257\varphi^{1/3}\mu(\varphi), & 0.003375 \leq \varphi \leq 0.05, \end{cases} \tag{5}$$

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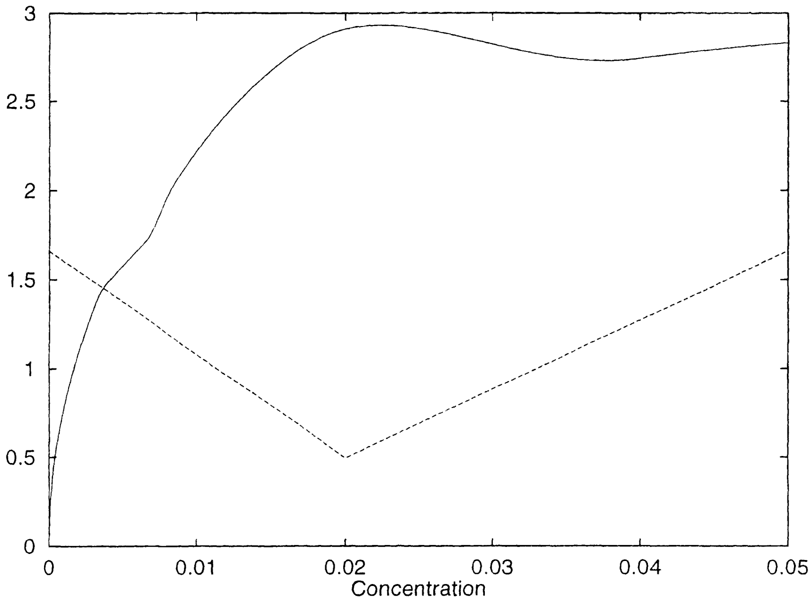

Figure 2: Dependence of the parameters σ_v(———), in cm/min, and β(– – –), in min^{-1}, on the solids fraction φ.

is plotted in Figure 2. The remaining parameter, β (the reciprocal of the correlation time [3]), is also shown in Figure 2. Not enough is known about β to represent its dependence precisely. Figure 2 is consistent with the limited data available. The small value of $\beta(0.02)$ reflects the persistence of velocities at that concentration [3]. By using the Markov model to interpret the phenomena occurring in suspensions, we hope to aid in the design of new experiments that will provide more accurate values of the parameters.

Formally, eqn (2) is a linear first-order differential equation whose solution contains an infinite series of time-dependent Gaussian random variables. Honeycutt [7,14,15] truncated the formal solutions of eqns (1) and (2) and matched both the deterministic and stochastic parts. Thus, the time-dependent Gaussian random variables are replaced by algebraic terms with the correct time-dependence and random variables that are independent of time. Honeycutt sets out the solution in such a way that the stochastic terms are given by Gaussian random variables ψ_1 and ψ_2 with $E(\psi_i) = 0$ and $E(\psi_i\psi_j) = \delta_{ij}$. This requires matching the means, variances and covariances of the original stochastic variables with those of their replacements. The resulting fourth-order stochastic Runge-Kutta method is very efficient.

Use eqn (4) and let φ_i be the solids fraction in the cylindrical slice containing the test particle. Then

$$dV_k(t) = -\beta(\varphi_i)[V_k(t) - \mu(\varphi_i)]dt + [2\beta(\varphi_i)]^{1/2}\sigma_v(\varphi_i)dW_k \qquad (6)$$

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implies that the values of the three parameters are determined by the solids concentration in that thin slice [3]. (The three parameters are usually assumed to be functions of a concentration parameter that is a convolution of local concentrations with a Gaussian kernel [5,8], but a simpler assumption suffices for these suspensions. See Discussion.)

3 Simulation of sedimentation of entire suspensions

We simulated the sedimentation of a suspension with $\varphi = 0.02$ and compared our results to those predicted by Kynch's theory [10] and those obtained experimentally [4,10]. We used the following algorithm:

(i) Set the initial height $= H$.
(ii) Divide H into m sections (bins), each $h = H/m$ in height.
(iii) Place N particles randomly according to a uniform distribution over H. Record the number of particles, n_i, in each bin. The corresponding solids fraction is $\varphi_i = \varphi_0 n_i/n_0$ where φ_0 is the initial concentration and $n_0 = N/m$ is the mean number of particles in each bin.
(iv) Randomly choose an initial velocity for each particle from the 109 initial velocities measured by Tory and Pickard. Note that this velocity is independent of φ_i.
(v) Determine μ, σ_v and β from the equations used to generate Figures 1 and 2.
(vi) Choose Δt and move each particle the distance calculated from the fourth-order Runge-Kutta method. A particle that starts in a given bin is governed by the parameters for that bin even though it is in another bin at the end of the time interval. Record the position of each particle, but do not adjust the concentration of any bin until all particles have been moved.
(vii) For those particles that are in the lowest (active) bin, determine whether they would hit the packed bed. Count the particles that have settled out.
(viii) Reset the position of the packed bed. It takes $n_\infty = n_0\varphi_\infty/\varphi_0$ particles to pack a bin. Each particle that settles out raises the packed bed by h/n_∞.
(ix) After all particles have been moved, determine the new concentration in each bin. If some particles are still settling, go to step (v). If all particles have settled out, exit the program.

For the simulations reported here, we used $H = 1.23$ metres, $m = 100$, $\Delta t = 0.01$ minutes, $\varphi_0 = 0.02$ and $\varphi_\infty = 0.576$.

4 Results

Recently, Bürger and Tory [10] re-examined the data of Tory and Pickard [4] and used an extension of Kynch's theory to demonstrate the existence of an upper rarefaction wave in a suspension with $\varphi_0 = 0.02$. According

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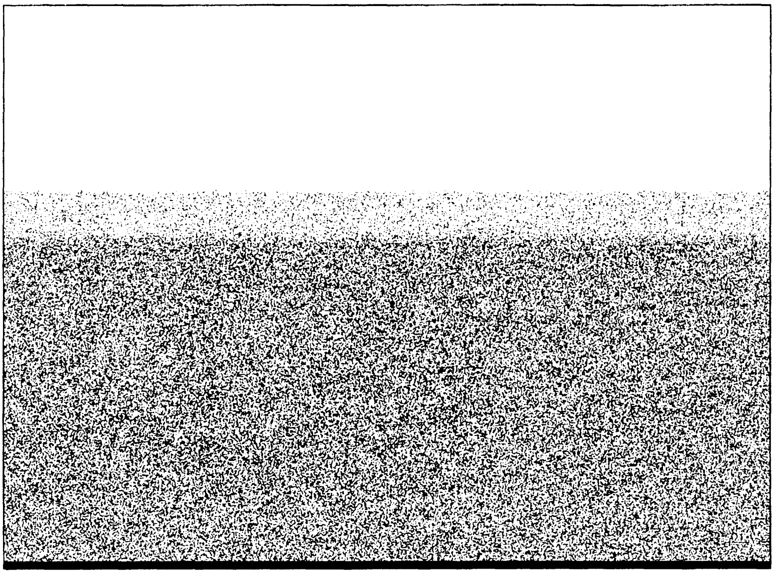

Figure 3: Spatial distribution of sphere centres at $t = 10$ minutes. Vertical positions were obtained from the simulation. Horizontal positions were assigned randomly to create a two-dimensional picture.

to their analysis, this region of reduced concentration is separated from the supernate and the bulk suspension by contact discontinuities. These jumps in φ and their propagation velocities are shown in Figure 1. As we move down the column, φ jumps from 0 to 0.0064, changes gradually to 0.00857 and then suddenly to 0.02. Figure 3 shows the corresponding changes in a simulation with $N = 200,000$. In the simulated suspension and in real suspensions of this concentration, both the interface and the concentration "discontinuity" are fuzzy, not sharp as predicted from Kynch's theory. Nevertheless, the region of reduced concentration is clearly delineated. Figure 3 also shows that the concentration in the bulk of the suspension, though uniform in the large, varies from point to point. Figure 4 shows how the concentration varies with height. This simulation started with two million particles, an average of 20,000 particles per bin. Apart from small fluctuations, the region just above the packed bed remains at the initial concentration of 0.02. (Fluctuations are much greater in simulations with only a small number of particles. See Discussion.) In real slurries, these random fluctuations arise initially from the mixing process and later from the variability of particle velocities. The simulation incorporates both of these. The Kynch gradient is visible in Figure 4, but there are other gradients that arise from the variability of particle velocity [5], i.e., from hydrodynamic diffusion [16]. However, these secondary gradients are so sharp that

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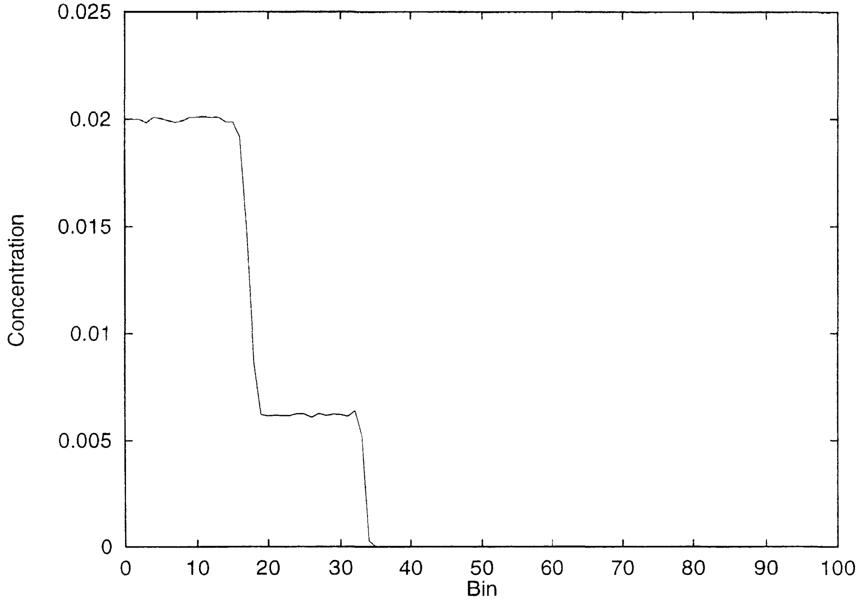

Figure 4: Variation of solids concentration with height at $t = 20$ minutes. The packed bed at the bottom is not shown.

they can be followed easily. Figure 5 shows how the positions of the interface and the sharp change in solids concentration vary with time. The interface falls at the rate of 3.326 bins per minute, which implies a velocity of -4.09 cm/min. The corresponding values for the concentration "discontinuity" are 4.101 bins per minute and -5.04 cm/min. These settling rates are close to the experimental values of -3.89 and -5.28 cm/min. and very close to the Kynch values of -4.08 and -5.08 cm/min obtained from Figure 1.

5 Discussion

There is some uncertainty in the experimental values obtained by Tory and Pickard [4] and re-analysed by Bürger and Tory [10] and considerably more freedom in interpreting the meaning of the interface velocities obtained by Verhoeven [10,11]. In constructing Figure 1, we used the estimated experimental concentrations of 0.0064 and 0.00857 to delineate the concentration gradient at the top of the suspension. Bürger and Tory used the experimental values of the rates of fall of the interface and the concentration "discontinuity". Though constructed on different bases, the two flux plots are very similar. The difference is much less than the experimental uncertainty in the data. Because the values of the parameters are not known precisely and because not all the relevant experimental measurements were made, the agreement between the theory and experiment is qualitative at this stage.

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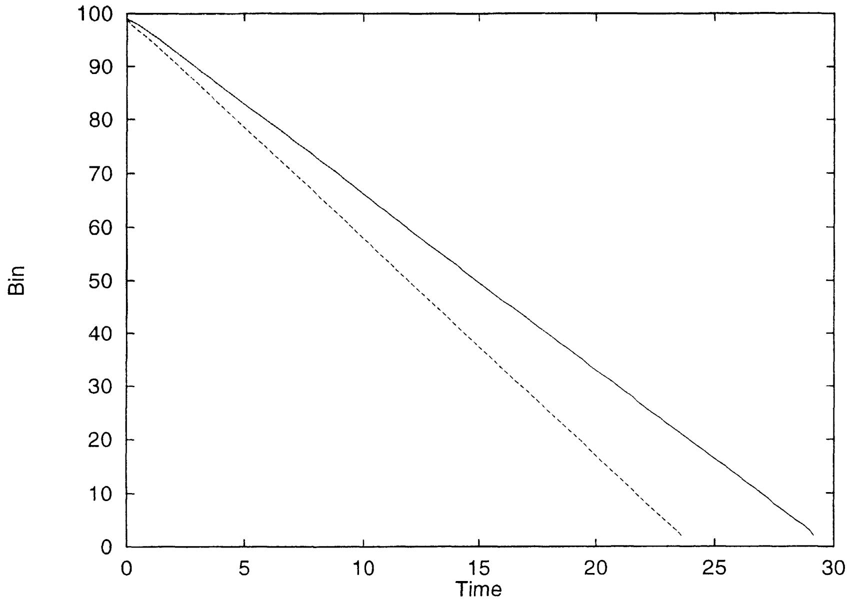

Figure 5: Evolution of solids concentration in a sedimenting suspension. The solid line represents the suspension-supernate interface and the dashed line the sharp change in solids concentration.

The purpose of the simulation was to compare results from the three-parameter Markov model with those obtained from Kynch's theory. In the sense that the rates of fall of the interface and the concentration "discontinuity" are essentially identical in the two treatments, the extended Kynch theory works perfectly. On the other hand, it is clear that the simulated results are much closer to reality. The suspension-supernate interface in Figure 3 is somewhat diffuse just like the interfaces observed by Tory and Pickard [4]. Also, in the simulation and in experiments, there is an induction period, during which the interface gradually becomes distinct. Aside from these points, there is a major conceptual advantage in using the Markov model. The Kynch assumption that identical particles at the same concentration have the same velocity is unrealistic and untrue. A key assumption of the Markov model is that the expected value of the steady-state velocity is the same for identical particles [5,8]. The model also predicts that these velocities will be normally distributed and the autocorrelation of velocities will decay exponentially. These predictions have been confirmed experimentially and computationally [3]. Realistic, mild conditions on σ_v and β as $\varphi \to 0$ are sufficient to guarantee that an interface will form at the top of a sedimenting suspension [17].

Solids profiles such as that in Figure 4 can also be obtained by solving the parabolic partial differential equation that includes the terms in the

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hyperbolic p.d.e. for Kynch sedimentation [9] and a term arising from hydrodynamic diffusion. The diffusion approach followed the Markov model by a decade [16,18], but has become more widely used. However, the earlier approach has two advantages over the later. First, velocities are continuous in the Markov model (and in reality), but not in the hydrodynamic-diffusion approach, which is based on the analogy to Fickian diffusion [18]. Second, simulations and experiments use similar numbers of particles and are subject to similar fluctuations in concentration. However, these fluctuations can cause problems in simulations and must be handled carefully [5,8]. In real slurries, locally dense regions will settle more quickly than those regions that are less dense than average. This effect is not incorporated in the simulation, but mean velocity varies only slightly for $0 < \varphi \leq 0.025$ and flux increases in this range. This prevents fluctuations from growing out of control provided that the number of particles is reasonably large ($n_0 \geq 2000$) and the time steps are small (0.01 minutes). A run using these values requires 52 minutes of computing time with a Pentium Pro 200 MHz system running Linux compared to 29.4 minutes for the simulated experiment. As faster computation and increased capacity become more readily available, larger and more elaborate simulations will be feasible.

References

[1] Kynch, G.J. A theory of sedimentation. *Transactions of the Faraday Society* **48**, pp. 166–176, 1952.

[2] Tory, E.M., Kamel, M.T. & Chan Man Fong, C.F. Sedimentation is container-size dependent. *Powder Technology* **73**, pp. 219–238, 1992.

[3] Tory, E.M. & Hesse, C.H. Theoretical and experimental evidence for a Markov model for sedimentation (Chapter 8). *Sedimentation of Small Particles in a Viscous Fluid*, ed. E.M. Tory, Computational Mechanics Publications: Southampton and Boston, pp. 241–281, 1996.

[4] Tory, E.M. & Pickard, D.K. A three-parameter Markov model for sedimentation. *Canadian Journal of Chemical Engineering* **55**, pp. 655–665, 1977.

[5] Pickard, D.K. & Tory, E.M. A Markov model for sedimentation: Fundamental issues and insights. *Advances in the Statistical Sciences, Vol. IV, Stochastic Hydrology*, eds. I.B. MacNeill & G.J. Umphrey, D. Reidel: Dordrecht, pp. 1–25, 1987.

[6] Pickard, D.K., Tory, E.M., & Tuckman, B.A. A three-parameter Markov model for sedimentation II. Simulation of transit times and comparison with experimental results. *Powder Technology* **49**, pp. 227–240, 1987.

[7] Tory, E.M., Bargiel, M. & Honeycutt, R.L. A three-parameter Markov model for sedimentation III. A stochastic Runge-Kutta method for computing first-passage times. *Powder Technology* **80**, pp. 133–146, 1994.

[8] Hesse, C.H. & Tory, E.M. The stochastics of sedimentation (Chapter 7). *Sedimentation of Small Particles in a Viscous Fluid*, ed. E.M. Tory,

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Computational Mechanics Publications: Southampton and Boston, pp. 199–239, 1996.

[9] Bustos, M.C., Concha, F., Bürger, R. & Tory, E.M. *Sedimentation and Thickening. Phenomenological Foundation and Mathematical Theory*, Kluwer: Dordrecht, pp. 111–148, 1999.

[10] Bürger, R. & Tory, E.M. On upper rarefaction waves in batch settling. *Powder Technology* **108**, 74-87, 2000.

[11] Verhoeven, J. Prediction of batch settling behaviour, B. Eng. thesis, McMaster University, 1963.

[12] Richardson, J.F. & Zaki, W.N. Sedimentation and fluidization. *Transactions of the Institution of Chemical Engineers* **32**, pp. 35–53, 1954.

[13] Segre, P.N., Herbolzheimer, E. & Chaikin, P.M. Long-range correlation in sedimentation. *Physical Review Letters* **79**, pp. 2574–2577, 1997.

[14] Honeycutt, R.L. Stochastic Runge-Kutta algorithms. I. White noise. *Physical Review A* **45**, pp. 600–603, 1992.

[15] Honeycutt, R.L. Higher order algorithms for the numerical integration of stochastic differential equations, Ph. D. thesis, Georgia Institute of Technology, 1990.

[16] Davis, R.H. Hydrodynamic diffusion of suspended particles: a symposium. *Journal of Fluid Mechanics* **310**, pp. 325–335, 1996.

[17] Tory, E.M. and Pickard. D.K. Extensions and refinements of a Markov model for sedimentation. *Journal of Mathematical Analysis and Applications* **86**, pp. 442–470, 1982.

[18] Ham, J.M. & Homsy, G.M. Hindered settling and hydrodynamic dispersion in quiescent sedimenting suspensions. *International Journal of Multiphase Flow* **14**, pp. 533–546, 1988.