Probabilistic Settling in the Local Exchange Model of Turbulent Particle Transport

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1 Introduction

Transport of particles by turbulent water or air plays an important role in a variety of ecological processes in freshwater, marine, and terrestrial environments. The particles involved may be living or nonliving, and may be transported passively or (if living) with different degrees of behavioral control. Examples include dispersal of microorganisms, invertebrates, larvae, and seeds or spores in freshwater, marine, and terrestrial ecosystems; transfer of suspended fine particulate organic matter (FPOM) to benthic suspension feeders in freshwater and marine ecosystems; spiraling of particle-bound nutrients in stream ecosystems; and the transport, fate, and ecological effects of particle-bound anthropogenic toxicants in freshwater and marine ecosystems (see McNair and Newbold 2001 for a concise review and references to the literature).

The Local Exchange Model (LEM) is a stochastic diffusion model of the transport of individual particles in turbulent flowing water. It was developed in a series of papers by McNair et al. (1997), McNair (2000), McNair and Newbold (2001), and McNair (2006) and was intended for application mainly to particles of neutral or near-neutral buoyancy that are strongly influenced by turbulent eddies. Turbulence can rapidly transfer such particles to the bed, where settlement can then occur by, for example, sticking to biofilms (e.g., FPOM, bacteria) or attaching to the substrate behaviorally (e.g., benthic invertebrates). Gravitational assistance may facilitate these processes but is not required. Thus, neutrally or even positively buoyant particles can settle at significant rates.

McNair et al. (1997) distinguished four key problems of turbulent transport in streams: (1) the entrainment problem, dealing with how particles are entrained into the water column from the bed; (2) the travel-time problem, dealing with how long entrained particles remain in the water column before hitting the bed; (3) the travel-distance problem, dealing with how far entrained particles are transported before hitting the bed; and (4) the settlement problem, dealing with how entrained particles settle (i.e., hit the bed and remain there for a positive length of time instead of reflecting back into the water column).

The need to distinguish between hitting the bed and actually settling was illustrated by McNair and Newbold (2001). They applied the LEM to data of Cushing et al. (1993), which deal with settling by FPOM in two Idaho streams (Smiley Creek and Salmon River). Cushing et al. collected natural FPOM by filtering stream water, then labeled it with ¹⁴C and injected it back into the streams. They monitored the water-column concentration of labeled FPOM at several sampling stations downstream from the injection point as the pulse of labeled FPOM was transported by the current. By integrating the measured concentration-versus-time curve for each station, they determined the amount of injected FPOM still in the water column when the pulse passed the station and, by difference, the amount that had settled.

The proportion of injected FPOM still in the water column as the pulse passed a given sampling station provides an estimate of the proportion of particles with settling distances greater than the station's distance from the injection point. Thus, the sequence of downstream station distances (independent variable) and corresponding proportions of labeled FPOM that had not yet settled (dependent variable) characterize the empirical survival function (or complementary cumulative distribution function) for the settling distance. Figure 1 shows data for Smiley Creek, together with the hitting-distance survival function predicted by the LEM (from McNair and Newbold, 2001, slightly modified). As the figure makes clear, actual settling distances tend to be much greater than predicted hitting distances. This is the result expected if particles typically hit the bed and immediately reflect back into the water column one or more times before settling.



Figure 1. Settling of fine particulate organic matter (FPOM) in Smiley Creek, Idaho, in July 1990. Data points represent the proportions of ¹⁴C-labeled FPOM that had not yet settled (vertical axis) at various distances downstream from the injection point (horizonatal axis). Together, they represent the empirical survival function (or complementary cumulative distribution function) for the settling distance. The dashed curve is the theoretical survival function for the hitting distance predicted by the Local Exchange Model (from McNair and Newbold, 2001, slightly modified). Note that the observed settling distances tend to be much greater than the predicted hitting distances. Data were estimated from Figure 3 of Cushing et al. (1993). See text for additional details.

Prior to publication of the results of McNair (2006), the LEM had been developed only to address hitting times and distances. McNair (2006) extended and generalized the results of all prior papers on the LEM, showing how to address hitting times, hitting distances, settling times, settling distances, and various other properties (e.g., total energy expended by an invertebrate larva during transport) in a single, unified framework. The main purpose of the present document is to summarize the results of McNair (2006); additional discussion and technical details can be found in that paper.

2 An overview of the Local Exchange Model

We now briefly outline the main ideas underlying the LEM as background for the model development to follow. A more-detailed discussion of the model can be found in McNair et al. (1997), including its derivation, relevant background material from fluid mechanics and the theory of stochastic diffusion processes, and literature references.

A wide variety of approaches are available for modeling particle transport by turbulent fluids. Options one must consider in choosing an approach include whether to use a continuous or discrete time parameter, whether to use a continuous or discrete state space, whether to pose a stochastic or deterministic model, whether to pose a particulate model (which explicitly represents the particulate nature of the substance being transported) or a continuum model (which suppresses the particulate nature of the substance and substitutes a spatially smoothed concentration function), and, if a particulate model is posed, whether to model a single particle or an ensemble of particles. Together, these options imply a large number of alternative model types. Several of these types have, in fact, been employed in the literature, but the overwhelming majority of particle-transport models are continuous-time, continuous-space, deterministic, continuum models that address ensembles of particles and assume their spatially smoothed concentration changes continuously through time by a combination of advection and Fickian diffusion. The basic modeling tool under this approach is the classical advection-diffusion equation, which is a parabolic partial differential equation that predicts the spatial dynamics of concentration.

In contrast, the LEM is a continuous-time, continuous-space, stochastic, particulate model that addresses a single particle. It predicts dynamics of the probability distribution and moments of the particle's changing spatial position, and also predicts the probability distribution and moments of various other properties of interest, such as the travel time or distance until the particle hits or settles on the bottom for the first time. Under this approach, the analogue of the deterministic advection-diffusion equation is the forward Kolmogorov equation (see below). It, too, is a parabolic partial differential equation and thus enjoys the same convenient analytical and computational properties as the advection-diffusion equation. However, the forward Kolmogorov equation governs the probability distribution of a single particle's spatial position rather than the (smoothed) spatial distribution of an ensemble of particles. The main advantage of this approach is that a variety of inherently probabilistic questions regarding the fate of individual particles can be posed and answered in a clear, natural, and reasonably simple manner.

The LEM is a stochastic diffusion model and therefore characterizes the spatial dynamics of a suspended particle as a continuous-time, continuous-space Markovian stochastic process with continuous sample paths. It can be derived, however, by first posing a discrete-time, discrete-space random-walk model and then passing to a continuous limit, as in McNair et al. (1997). The key ideas underlying the LEM are clearest in this discrete model.

We think of the water column as comprising discrete "packets" of water that move vertically as well as longitudinally. (As in the similar line of reasoning in classical fluid dynamics regarding vertical transfer of momentum, the physical dimensions of these notional packets are immaterial, since they approach zero in the limiting operation that produces the stochastic diffusion process.) Net longitudinal motion (e.g., driven by gravity and bed slope in streams) produces directional flow, which produces shear, which in turn produces turbulence. Vertical motion of packets is due primarily to turbulent mixing. The LEM includes sufficient fluid-mechanical mechanisms to predict the vertical profiles of current velocity and mixing.

The LEM obeys the Principle of Local Exchange, which asserts that the expected number of fluid packets moving upward and downward across any level of the water column during any instant of time must be equal (McNair et al., 1997). This principle ensures there is no compression or net vertical transport of water.

A suspended particle is viewed as a point that occurs within a fluid packet. During any instant of time, a particle may move vertically either by being carried along with a packet, by Brownian motion, by behavioral means (for motile organisms), or by sinking (including "negative sinking", if positively buoyant). As noted above, the model addresses a single focal particle, and it must therefore be assumed that interactions with other suspended particles either do not occur or have a negligible effect on the focal particle.

Consider a water body of constant depth H, and let u(z) denote the current velocity at elevation $z \ (0 \le z \le H)$. Let Z(t) denote a suspended particle's elevation above the bottom at time $t \ge 0$, with $Z(0) = z_0 \in (0, H]$. Fluid eddies, molecular collisions, and (in the case of motile organisms) body or appendage movements cause the particle to move up and down, so that its elevation changes irregularly. It is therefore reasonable to suppose that $\{Z(t); t \ge 0\}$ is a stochastic diffusion process. Let $f(z_0; t, z)dz$ denote the probability that $Z(t) \in (z, z + dz)$, given $Z(0) = z_0$. Then $f(z_0; t, z)$ is the probability density function of Z(t) and is governed by the so-called forward and backward Kolmogorov equations. The forward equation is

$$\frac{\partial f}{\partial t} + \frac{\partial(\mu f)}{\partial z} - \frac{1}{2} \frac{\partial^2(\nu f)}{\partial z^2} = 0, \quad t > 0, \ 0 < z < H, \tag{1}$$

where $\mu(z)$ and $\nu(z) > 0$ are the infinitesimal mean and infinitesimal variance. Both $\mu(z)$ and $\nu(z)$ are time-homogeneous in the LEM, so the backward equation can be written as

$$\frac{\partial f}{\partial t} - \mu(z_0)\frac{\partial f}{\partial z_0} - \frac{1}{2}\nu(z_0)\frac{\partial^2 f}{\partial z_0^2} = 0, \quad t > 0, \ 0 < z_0 < H.$$

$$\tag{2}$$

The LEM is characterized by the following special forms for the infinitesimal mean and variance:

$$\mu(z) = K'(z) - s$$

$$\nu(z) = 2K(z),$$
(3)

where s is the particle's advective vertical velocity component (e.g., the fall velocity of a nonmotile particle, with s > 0 implying positive sinking or negative buoyancy) and K(z) is the dispersion coefficient of vertical motion. (Note: throughout this document, a single prime (') denotes the first derivative of a function with respect to its argument and a double prime (") denotes the second derivative.) These forms are derived in McNair et al. (1997) and ensure compliance with the Principle of Local Exchange.

Three processes may contribute to the vertical dispersion coefficient: (1) Brownian motion, (2) nondirected motility (behavioral kinesis) of living organisms, and (3) vertical movements of water due to turbulent eddies. The contribution of the first two processes to vertical particle dispersion can be represented by a single particle diffusion coefficient D. (Note: early papers on the LEM expressed the contribution of the first two processes by a proportionality constant times the kinematic molecular viscosity of water, but it seems preferable to employ an explicit particle diffusion coefficient.) The contribution of the third process is controlled by the kinematic eddy viscosity $l(z)^2 du/dz$ and the particle's responsiveness to the motion of eddies, with l(z) being Prandtl's mixing length. Thus, the vertical dispersion coefficient in the LEM has the form,

$$K(z) = D + \psi l(z)^2 \frac{\mathrm{d}u}{\mathrm{d}z},\tag{4}$$

where ψ is a nonnegative constant representing the degree to which particle motion responds to turbulence. The value of ψ should depend on the ratio of the characteristic length scale of turbulent

eddies to the characteristic particle length scale, and on the ratio of the density of water to the particle density, with high (low) ratios producing a large (small) coefficient. However, we are not aware of any formulas expressing ψ in terms of such underlying properties.

We assume Prandtl's mixing length l(z) has the following functional form, which is widely used in advection-dispersion models of rivers (additional forms are considered by McNair et al., 1997):

$$l(z) = \kappa z \sqrt{1 - z/H}.$$
(5)

Here, $\kappa \approx 0.4$ (dimensionless) is Von Kármán's "constant" (heavy suspended sediment loads can reduce κ by half: Vanoni and Nomicos, 1960; Richards, 2004).

Using this functional form for l(z), current velocity u(z) is determined by the differential equation,

$$\frac{\mathrm{d}u}{\mathrm{d}z} = \frac{1}{2l(z)^2} \left[-M + \sqrt{M^2 + 4l(z)^2 u_*^2 (1 - z/H)} \right]$$
(6)

$$= \frac{2u_*^2(1-z/H)}{M + \sqrt{M^2 + [2\kappa u_* z(1-z/H)]^2}}$$
(7)

for $0 < z \leq H$, with initial condition u(0) = 0 (McNair et al., 1997, Eq. (12)). Parameter $M \approx 10^{-6}$ m² s⁻¹ is the kinematic molecular viscosity of water, and $u_* = \sqrt{\tau_0/\rho}$ is the bed shear velocity, where τ_0 is bed shear stress and ρ is the density of water. The formulation for τ_0 used by McNair et al. (1997), McNair (2000), and McNair and Newbold (2001) yields the following classical expression for u_* in rivers and streams:

$$u_* = \sqrt{gH\sin(\theta)},\tag{8}$$

where g is the gravitational acceleration constant and θ is the longitudinal angle of the bed. McNair et al. (1997) applied the LEM to data of Vanoni (1953) for a laboratory flume with a sand bed and found that Eqs. (7) and (8) accurately predicted the velocity profile in experimental runs where dune development was not significant.

The vertical dispersion coefficient can now be written as follows:

$$K(z) = D + \frac{\psi}{2} \left\{ -M + \sqrt{M^2 + [2\kappa u_* z(1 - z/H)]^2} \right\}.$$
(9)

Thus, K(z) is finite and positive, is roughly parabolic, and achieves its minimum value (= D > 0)at z = 0 and z = H and its maximum value $(= D + 0.5\psi[-M + \sqrt{M^2 + (0.5\kappa u_*H)^2}])$ at z = H/2. The rate of vertical dispersion is determined mainly by D near the bottom and the surface but mainly by $\psi \kappa u_* H$ away from these boundaries (assuming $D, M \ll \psi \kappa u_* H$).

3 The settling time and settling distance

The hitting-time and hitting-distance problems deal with the time and distance a particle travels until it encounters the bottom for the first time; whether the particle settles (i.e., remains on the bottom for a positive length of time) or immediately reflects back into the water column upon encounter is irrelevant. We may characterize this situation by saying that every particle is always in exactly one of two states: 0 if it has not yet encountered the bottom, and 1 if it has. Any particle with initial elevation Z(0) > 0 begins in state 0, and its state switches to 1 at the instant it encounters the bottom, regardless of whether it settles or reflects. In effect, then, a particle in state 0 is absorbed by the bottom upon encounter and is immediately replaced by a particle in state 1. The bottom therefore functions as an absorbing barrier in the context of this problem. We are now interested in the time and distance a particle travels until it settles for the first time, taking into account the possibility that it may encounter the bottom and immediately reflect back into the water column multiple times before settling. In this case, encountering the bottom is not enough to terminate a particle trajectory: a second stochastic event, co-occuring with encounter, determines whether the trajectory terminates (the particle settles) or continues (the particle reflects back into the water column). This type of behavior at the bottom requires a different type of boundary condition that is neither absorbing nor reflecting.

In this section, we present equations governing the distribution and moments of the settling time and settling distance. We do this by developing a conceptual framework that is sufficiently general to include the hitting-time, hitting-distance, settling-time, and settling-distance problems (among others) as special cases. As the basis for this approach, we begin by introducing the concept of the total cost of a particle trajectory. We emphasize that by "cost", we simply mean something that accrues during transport (e.g., time spent in transit, distance transported, energy expended in transit, etc.). No negative connotation is intended, and we could equally well have used the term "benefit" or "reward".

3.1 The total cost of a particle trajectory

As noted above, the LEM assumes that a particle's elevation $\{Z(t); t \ge 0\}$ is a stochastic diffusion process. Suppose that, as the particle moves up and down, it accrues a cost at a rate (per unit time) that is a continuous function of its present elevation Z(t). Let r(Z(t)) denote the cost-accrual rate. If the particle's trajectory terminates at some time T^* (e.g., when it first encounters the bottom, or when it settles, depending on the problem of interest), then the total cost accrued over the entire trajectory is simply the integral of r(Z(t)) between t = 0 and $t = T^*$. Thus, given that $Z(0) = z_0$, the total cost $C(z_0)$ of the trajectory is given by

$$C(z_0) = \int_0^{T^*(z_0)} r(Z(t)) \,\mathrm{d}t,\tag{10}$$

where existence of the integral is assured by continuity of Z(t) and $r(\cdot)$.

Some examples will illustrate the flexibility of the concept of a trajectory's total cost. To begin, suppose we focus on time spent in transit as the cost of interest. We therefore choose r(z) = 1in Eq. (10), since time in transit accrues at unit rate. Suppose further that we are interested in trajectories terminated by hitting the bed for the first time. Let $T_H(z_0)$ denote the hitting time of a particle whose initial elevation is z_0 , and let $T^* = T_H(z_0)$ in Eq. (10). Then the total cost is given by

$$C(z_0) = \int_0^{T_H(z_0)} \mathrm{d}t = T_H(z_0), \tag{11}$$

which is simply the hitting time. Alternatively, suppose we are interested in trajectories terminated by settling on the bed rather than just hitting it (while continuing to focus on time spent in transit as the cost). Letting $T_S(z_0)$ denote the settling time of a particle whose initial elevation is z_0 and letting $T^* = T_S(z_0)$ in Eq. (10), we find that the total cost is given by Eq. (11) with $T_H(z_0)$ replaced by $T_S(z_0)$. In this case, then, the total cost is simply the settling time.

Now suppose we focus on distance transported as the cost. We therefore choose r(z) = u(z)in Eq. (10), where u(z) is the current velocity at elevation z. If we are interested in trajectories terminated by hitting the bed for the first time, we let $T^* = T_H(z_0)$ and the total cost is given by

$$C(z_0) = \int_0^{T_H(z_0)} u(Z(t)) \,\mathrm{d}t,\tag{12}$$

which is the longitudinal distance the particle travels before hitting the bed for the first time; i.e., the hitting distance, which we may denote by $D_H(z_0)$. On the other hand, if we are interested in trajectories terminated by settling on the bed (with transport distance as the cost), we let $T^* = T_S(z_0)$ and the total cost is given by Eq. (12) with $T_H(z_0)$ replaced by $T_S(z_0)$. In this case, then, the total cost is the longitudinal distance the particle travels before settling on the bed. This is the settling distance, which we may denote by $D_S(z_0)$.

More broadly, r(z) can represent the rate of almost any process of interest. For example, if we were interested in metabolic costs incurred by a benchic invertebrate during transport, we might choose r(z) to represent its rate of energy expenditure or oxygen consumption. In the present paper, however, we will only consider time and distance costs.

3.2 Distribution of the total cost

Let $\mathcal{G}(\xi, z_0)$ denote the survival function for the total cost $C(z_0)$ of a particle trajectory; that is,

$$\mathcal{G}(\xi, z_0) = P\{C(z_0) > \xi\}.$$

Then $\mathcal{G}(\xi, z_0)$ is governed by the following linear parabolic partial differential equation:

$$r(z_0)\frac{\partial \mathcal{G}}{\partial \xi} - [K'(z_0) - s]\frac{\partial \mathcal{G}}{\partial z_0} - K(z_0)\frac{\partial^2 \mathcal{G}}{\partial z_0^2} = 0, \quad \xi > 0, \ 0 < z_0 < H$$
(13)

(see McNair, 2006).

We must supplement Eq. (13) with an initial condition at $\xi = 0$ and with boundary conditions at $z_0 = 0$ and $z_0 = H$. The initial condition is

$$\mathcal{G}(0, z_0) = 1, \qquad 0 < z_0 < H.$$
 (14)

As in the hitting-time and hitting-distance problems, we assume the upper boundary is reflecting. The appropriate boundary condition at $z_0 = H$ is therefore

$$\left[\partial \mathcal{G}/\partial z_0\right]_{z_0=H} = 0, \qquad \xi > 0 \tag{15}$$

(see McNair, 2006).

The form of the lower boundary condition differs from that in the hitting-time and hittingdistance problems, where $z_0 = 0$ is absorbing (in which case $\mathcal{G}(\xi, 0) = 0$). We now wish to allow probabilistic settling, where a particle encountering the bottom can either settle or reflect back into the water column, each with positive probability.

The basic idea behind our approach is easiest to see in a discretized form of the diffusion model, where we assume a time step of size τ and a (vertical) distance step of size δ . A particle at elevation δ (one step above the bottom) moves up with probability $p(\delta, \tau)$, down with probability $q(\delta, \tau)$, and fails to move with probability $1 - p(\delta, \tau) - q(\delta, \tau)$. If it moves down, it encounters the bottom, in which case it either settles (i.e., remains on the bottom for a positive length of time) with probability $\pi_0(\delta, \tau)$ or immediately reflects back to δ with probability $1 - \pi_0(\delta, \tau)$. Allowing $\delta, \tau \to 0$ in an appropriate manner yields the following boundary condition at $z_0 = 0$:

$$\left[\partial \mathcal{G}/\partial z_0\right]_{z_0=0} = Q_0 \mathcal{G}(\xi, 0), \qquad \xi > 0, \tag{16}$$

where Q_0 is a positive constant with dimensions of Length⁻¹(see Appendix A).

In the stochastic process literature, a boundary with this type of condition is sometimes called an elastic boundary (e.g., Mandl, 1968). We find the terms "leaky boundary" and "porous boundary"

more evocative and will use the former throughout this paper. Thus, Eq. (16) is the boundary condition for a leaky boundary. Intuitively, we think of settling occurring if a particle finds a "leak" in the lower boundary (e.g., a microsite with sufficiently low shear stress or other sufficiently favorable properties) when it encounters the bottom; otherwise, the particle reflects back into the water column. Coefficient Q_0 is a measure of how leaky the boundary is. In the limit as $Q_0 \to 0$, we obtain the condition for a reflecting boundary (i.e., $[\partial \mathcal{G}/\partial z_0]_{z_0=0} = 0$), which corresponds to absolutely no leak and, hence, certain reflection upon encounter. In the limit as $Q_0 \to \infty$, we obtain the condition for an absorbing boundary (i.e., $\mathcal{G}(\xi, 0) = 0$; this is easiest to see if we divide Eq. (16) by Q_0 before passing to the limit), which corresponds to an infinitely leaky boundary and, hence, certain settling upon encounter. It is apparent, then, that a leaky boundary includes both reflecting and absorbing boundaries as limiting special cases and is therefore a more-general type of boundary.

The fact that Q_0 is constant implies that the leakiness of the lower boundary does not change with time, and hence that (like properties of the flow) the availability of suitable settlement sites is approximately constant. In practice, this means either that there is no temporal trend of net deposition or erosion of particles that occupy the same types of settlement sites, or that any such trend is not sufficiently pronounced to significantly alter the availability of potential settlement sites over the period of interest (e.g., a period with duration equal to the 95th or 99th percentile of the distribution of particle settling times). The assumption of constant Q_0 is usually plausible in highly turbulent natural streams with extensive riffles or other types of nondepositional reaches (e.g., Smiley Creek, Idaho: see Figure 1).

For realistic choices of vertical dispersion function K(z), Eq. (13) must be solved numerically. The probability density function $g(\xi, z_0)$ can then be computed by numerically differentiating the survival function, using the fact

$$g(\xi, z_0) = -\mathrm{d}\mathcal{G}(\xi, z_0)/\mathrm{d}\xi.$$

Other useful properties of the total cost distribution that are easily computed from the survival function include the median, quantiles, and interquartile range.

3.3 Moments of the total cost

Equations governing the mean and higher moments of the total cost of a particle trajectory are easily deduced from the above partial differential equation and boundary conditions for the survival function. Let $m_i(z_0)$ denote the *j*-th moment of the total cost; i.e.,

$$m_j(z_0) = E[C(z_0)^j], \qquad j = 0, 1, 2, \dots$$

(where $E[\cdot]$ denotes mathematical expectation), with $m_0(z_0) = 1$. Following McNair (2000), we multiply Eq. (13) and its boundary conditions by $j\xi^{j-1}$, then integrate over $0 < \xi < \infty$. Using the fact that

$$j \int_0^\infty \xi^{j-1} \mathcal{G}(\xi, z_0) \,\mathrm{d}\xi = E[C(z_0)^j], \qquad j = 1, 2, 3, \dots,$$

we find that

$$K(z_0)m''_j + [K'(z_0) - s]m'_j = -jr(z_0)m_{j-1}, \quad 0 < z_0 < H; m'_i(0) = Q_0m_i(0), \quad m'_i(H) = 0$$
(17)

for j = 1, 2, 3, ..., where $m_{j-1}(z_0)$ is presumed known. This is a sequence of linear two-point boundary-value problems, where the *j*-th is solved before proceeding to the (j + 1)-th.

The standard deviation $\sigma(z_0)$ of the total cost distribution is a useful measure of dispersion and is easily computed from the first two moments as

$$\sigma(z_0) = \sqrt{m_2(z_0) - m_1(z_0)^2}.$$

3.4 The settling time

A particle's settling time $T_S(z_0)$ is the amount of time that has elapsed when the particle settles for the first time, given that it started at elevation z_0 . A particle that has settled may subsequently become resuspended, so a given particle may settle more than once. The settling time, however, applies only to the first settling event from a specified initial elevation.

Equations governing the distribution and moments of settling time $T_S(z_0)$ are deduced from Eqs. (13) and (17) by choosing $r(z_0) = 1$ and setting $\xi = t$, where t denotes time. Thus, the survival function is governed by

$$\frac{\partial \mathcal{G}}{\partial t} - [K'(z_0) - s] \frac{\partial \mathcal{G}}{\partial z_0} - K(z_0) \frac{\partial^2 \mathcal{G}}{\partial z_0^2} = 0, \quad t > 0, \ 0 < z_0 < H,$$
(18)

subject to initial condition (14) and boundary conditions (15) and (16). The moments are governed by the sequence of boundary-value problems,

$$K(z_0)m''_j + [K'(z_0) - s]m'_j = -jm_{j-1}, \quad 0 < z_0 < H; m'_j(0) = Q_0m_j(0), \quad m'_j(H) = 0$$
(19)

for $j = 1, 2, 3, \ldots$, with $m_0(z_0) = 1$.

3.5 The settling distance

A particle's settling distance $D_S(z_0)$ is the longitudinal distance the particle has traveled when it settles for the first time, given an initial elevation of z_0 . As in the case of the settling time, a particle may settle more than once, but the settling distance applies only to the first settling event from a specified initial elevation.

Equations governing the distribution and moments of settling distance $D_S(z_0)$ are deduced from Eqs. (13) and (17) by choosing $r(z_0) = u(z_0)$ and setting $\xi = x$, where $u(z_0)$ is the current velocity at elevation z_0 and x denotes longitudinal distance downstream. The survival function is therefore governed by

$$u(z_0)\frac{\partial \mathcal{G}}{\partial x} - [K'(z_0) - s]\frac{\partial \mathcal{G}}{\partial z_0} - K(z_0)\frac{\partial^2 \mathcal{G}}{\partial z_0^2} = 0, \quad x > 0, \ 0 < z_0 < H,$$
(20)

subject to initial condition (14) and boundary conditions (15) and (16), while the moments are governed by the sequence of boundary-value problems,

$$K(z_0)m''_j + [K'(z_0) - s]m'_j = -ju(z_0)m_{j-1}, \quad 0 < z_0 < H; m'_i(0) = Q_0m_i(0), \quad m'_i(H) = 0$$
(21)

for $j = 1, 2, 3, \ldots$, with $m_0(z_0) = 1$.

3.6 Settling versus hitting

We noted above that the parameter Q_0 appearing in the boundary condition at $z_0 = 0$ is a measure of how leaky the lower boundary is, and that a leaky boundary becomes absorbing in the limit as $Q_0 \to \infty$. Since the only difference between the equations governing hitting problems and settling problems lies in the boundary condition imposed at $z_0 = 0$, all of the theory developed for the hitting-time and hitting-distance problems in earlier papers on the LEM can be deduced from results for the settling-time and settling-distance problems by allowing $Q_0 \to \infty$. Moreover, the differences between computed hitting and settling times, and between computed hitting and settling distances, become negligible at sufficiently large values of Q_0 (see below).

4 Numerical results

In the previous section, we extended the LEM to include probabilistic settling. Here we illustrate the main properties of the extended LEM by numerically analyzing the equations governing the distribution and moments of the settling time and distance. We then apply the model to the data of Cushing et al. (1993), discussed in the Introduction, to determine whether the LEM with probabilistic settling is able to predict a settling-distance distribution that matches the observed distribution more closely than does the predicted hitting-distance distribution.

4.1 The settling time

We begin by reducing the settling-time equations to dimensionless form. Let

$$\begin{split} \hat{t} &= t\psi\kappa u_*/H, \quad \hat{z} = z_0/H, \\ \hat{s} &= s/\psi\kappa u_*, \quad \hat{M} = M/\kappa u_*H, \\ \hat{Q} &= Q_0H, \quad \hat{D} = D/\psi\kappa u_*H, \\ \hat{K}(\hat{z}) &= K(\hat{z}H)/\psi\kappa u_*H, \quad \hat{l}(\hat{z}) = l(\hat{z}H)/\kappa H, \\ \hat{\mathcal{G}}(\hat{t}, \hat{z}) &= \mathcal{G}(\hat{t}H/\psi\kappa u_*, \hat{z}H), \quad \hat{g}(\hat{t}, \hat{z}) = g(\hat{t}H/\psi\kappa u_*, \hat{z}H)H/\psi\kappa u_*, \\ \hat{m}_j(\hat{z}) &= m_j(\hat{z}H)(\psi\kappa u_*/H)^j, \quad \hat{\sigma}(\hat{z}) = \sigma(\hat{z}H)\psi\kappa u_*/H. \end{split}$$

Then the vertical dispersion coefficient can be written in the following dimensionless form:

$$\hat{K}(\hat{z}) = \hat{D} + \frac{1}{2} \left\{ -\hat{M} + \sqrt{\hat{M}^2 + 4\hat{z}^2(1-\hat{z})^2} \right\}.$$
(22)

Similarly, the equation governing the survival function can be written in the dimensionless form,

$$\frac{\partial \hat{\mathcal{G}}}{\partial \hat{t}} - [\hat{K}'(\hat{z}) - \hat{s}] \frac{\partial \hat{\mathcal{G}}}{\partial \hat{z}} - \hat{K}(\hat{z}) \frac{\partial^2 \hat{\mathcal{G}}}{\partial \hat{z}^2} = 0, \quad t > 0, \ 0 < \hat{z} < 1,$$
(23)

subject to

$$\hat{\mathcal{G}}(0,\hat{z}) = 1, \quad 0 < \hat{z} < 1,$$
(24)

and

$$\left[\partial \hat{\mathcal{G}}/\partial \hat{z}\right]_{\hat{z}=0} = \hat{Q}\hat{\mathcal{G}}(\hat{t},0), \quad \left[\partial \hat{\mathcal{G}}/\partial \hat{z}\right]_{\hat{z}=1} = 0, \qquad \hat{t} > 0.$$
⁽²⁵⁾

The equations governing the moments can be written in the dimensionless form,

$$\hat{K}(\hat{z})\hat{m}''_{j} + [\hat{K}'(\hat{z}) - \hat{s}]\hat{m}'_{j} = -j\hat{m}_{j-1}, \quad 0 < \hat{z} < 1;
\hat{m}'_{j}(0) = \hat{Q}\hat{m}_{j}(0), \quad \hat{m}'_{j}(1) = 0$$
(26)

for $j = 1, 2, 3, \ldots$, with $\hat{m}_0(\hat{z}) = 1$.

The dimensionless equations governing the survival function and moments contain four parameters: \hat{D} , \hat{M} , \hat{s} , and \hat{Q} . These parameters, then, are the key determinants of the relationship between $\hat{\mathcal{G}}$ and its arguments \hat{t} and \hat{z} , and between \hat{m}_j and its argument \hat{z} . The roles of parameters \hat{s} and \hat{M} in determining the form of the settling-time distribution are qualitatively the same as their roles in determining the form of the hitting-time distribution, which were detailed by McNair (2000). We therefore restrict our attention here to the roles of \hat{z} and the two new parameters \hat{Q} and \hat{D} .

4.1.1 Survival and probability density functions

The only difference between the hitting-time and settling-time problems is the form of the boundary condition at the bed. Since this boundary condition for the settling-time problem approaches that for the hitting-time problem as $\hat{Q} \to \infty$, increasing \hat{Q} causes the survival and probability density functions for the settling time to converge to those for the hitting time, as illustrated in panels A and B of Figure 2. For any particular (finite) value of \hat{Q} , however, the survival probability for the settling time (i.e., the probability that the particle has not yet settled) is higher than that for the hitting time for all \hat{t} , as illustrated in panel A of Figure 2. The numerical examples also suggest that increasing the value of \hat{Q} has relatively little effect on the modal settling time, and that its main effect is to simultaneously increase the height of the mode and decrease the thickness of the upper tail of the settling-time distribution.

Increasing D tends to reduce the survival probability for all \hat{t} , increase the height of the mode of the settling-time distribution, decrease the thickness of the upper tail of the distribution, but change the position of the mode relatively little. These properties are illustrated in panels C and D of Figure 2.

The survival function is rather insensitive to dimensionless initial elevation \hat{z} , except for values of about 0.05 or less (panel E of Figure 2. Similarly, the shape of the probability density function is fairly insensitive to \hat{z} , except for values of about 0.25 or less (panel F). For very small values of \hat{z} (roughly 0.1 or less), a high, acute mode occurs at $\hat{t} \ll 1$, indicating an increased likelihood of settling almost immediately. In all cases, however, the probability density function retains a thick upper tail.

4.1.2 Mean and standard deviation

Vertical profiles of the dimensionless mean $\hat{m}_1(\hat{z})$ and standard deviation $\hat{\sigma}(\hat{z})$ of the setting time are shown in Figure 3. Panel A shows $\hat{m}_1(\hat{z})$ for the same series of increasing \hat{Q} used in Panel A of Figure 2, and it illustrates convergence (decrease) of the mean settling-time profile to the mean hitting-time profile with increasing \hat{Q} . Panel B shows $\hat{m}_1(\hat{z})$ for the same series of increasing \hat{D} used in Panel C of Figure 2, illustrating the decrease in mean settling time with increasing \hat{D} . Panel C shows the dimensionless mean (solid curves) and standard deviation (dashed curves) for three combinations of \hat{Q} and \hat{D} (listed in the figure caption), illustrating the fact that the standard deviation is relatively constant throughout most of the water column, changing rapidly only near the bed.



Figure 2. Effects of \hat{D} , \hat{Q} , and \hat{z} on the survival function and dimensionless probability density function of the settling time. $\hat{M} = 10^{-4}$ and $\hat{s} = 10^{-1}$ in all examples. A — The effect of \hat{Q} on survival function $\hat{\mathcal{G}}(\hat{t}, 0.75)$. Solid curves apply to the settling time for three choices of \hat{Q} ; the dashed curve shows the corresponding relationship for the hitting time. $\hat{D} = 10^{-6}$ in all four curves. Values of \hat{Q} in the solid curves are 10^3 (curve 1), 10^4 (curve 2), and 10^5 (curve 3). Note that the survival function for the settling time approaches that for the hitting time as \hat{Q} increases. B — The same as panel A, except that the corresponding probability density functions $\hat{g}(\hat{t}, 0.75)$ are shown. C — The effect of \hat{D} on survival function $\hat{\mathcal{G}}(\hat{t}, 0.75)$. $\hat{Q} = 10^3$ in all three curves. Values of \hat{D} are 10^{-6} (curve 1), 10^{-4} (curve 2), and 10^{-2} (curve 3). D — The same as panel C, except that the corresponding probability density functions $\hat{g}(\hat{t}, 0.75)$ are shown. E — The effect of \hat{z} on survival function $\hat{\mathcal{G}}(\hat{t}, \hat{z})$. $\hat{Q} = 10^3$ and $\hat{D} = 10^{-4}$ in all three curves. Values of \hat{z} are 0.95 (curve 1), 0.75, 0.50, 0.25, and 0.05 (curve 5). F — The same as panel E, except that the corresponding probability density functions $\hat{g}(\hat{t}, \hat{z})$ are shown.



Figure 3. Effects of \hat{D} and \hat{Q} on vertical profiles of the dimensionless mean $\hat{m}_1(\hat{z})$ and standard deviation $\hat{\sigma}(\hat{z})$ of the settling time. Each panel shows how $\hat{m}_1(\hat{z})$ or $\hat{\sigma}(\hat{z})$ (horizontal axis) varies with dimensionless elevation \hat{z} (vertical axis). $\hat{M} = 10^{-4}$ and $\hat{s} = 10^{-1}$ in all examples. A — The effect of \hat{Q} on $\hat{m}_1(\hat{z})$. Solid curves apply to the settling time for three choices of \hat{Q} ; the dashed curve shows the corresponding relationship for the hitting time. $\hat{D} = 10^{-6}$ in all four curves. Values of \hat{Q} in the solid curves are 10^3 (curve 1), 10^4 (curve 2), and 10^5 (curve 3). Note that $\hat{m}_1(\hat{z})$ for the settling time approaches that for the hitting time as \hat{Q} increases. B — The effect of \hat{D} on $\hat{m}_1(\hat{z})$. $\hat{Q} = 10^3$ in all three curves. Values of \hat{D} are 10^{-6} (curve 1), 10^{-4} (curve 2), and 10^{-2} (curve 3). C — Comparison of vertical profiles for the dimensionless mean (solid curves) and standard deviation (dashed curves) of the settling time for different choices of \hat{D} and \hat{Q} . Curve 1: $\hat{D} = 10^{-6}$, $\hat{Q} = 4 \times 10^3$. Curve 2: $\hat{D} = 10^{-6}$, $\hat{Q} = 10^4$. Curve 3: $\hat{D} = 10^{-2}$, $\hat{Q} = 10^4$. Note that, except for very close to the bed, the standard deviation is nearly constant over elevation.

4.2 The settling distance

To reduce the settling-distance equations to dimensionless form, let

$$\begin{split} \hat{x} &= x\psi\kappa^2/H, \quad \hat{z} = z_0/H, \\ \hat{s} &= s/\psi\kappa u_*, \quad \hat{M} = M/\kappa u_*H, \\ \hat{Q} &= Q_0 H, \quad \hat{D} = D/\psi\kappa u_*H, \\ \hat{K}(\hat{z}) &= K(\hat{z}H)/\psi\kappa u_*H, \quad \hat{l}(\hat{z}) = l(\hat{z}H)/\kappa H, \quad \hat{u}(\hat{z}) = u(\hat{z}H)\kappa/u_*, \\ \hat{\mathcal{G}}(\hat{x}, \hat{z}) &= \mathcal{G}(\hat{x}H/\psi\kappa^2, \hat{z}H), \quad \hat{g}(\hat{x}, \hat{z}) = g(\hat{x}H/\psi\kappa^2, \hat{z}H)H/\psi\kappa^2, \\ \hat{m}_i(\hat{z}) &= m_i(\hat{z}H)(\psi\kappa^2/H)^j, \quad \hat{\sigma}(\hat{z}) = \sigma(\hat{z}H)\psi\kappa^2/H. \end{split}$$

Then the vertical dispersion coefficient can again be written in dimensionless form (22), while the differential equation governing the vertical profile of current velocity can be written in the dimensionless form,

$$\frac{d\hat{u}}{d\hat{z}} = \frac{2(1-\hat{z})}{\hat{M} + \sqrt{\hat{M}^2 + 4\hat{z}^2(1-\hat{z})^2}}.$$
(27)

The equation governing the survival function can be written in the dimensionless form,

$$\hat{u}(\hat{z})\frac{\partial\hat{\mathcal{G}}}{\partial\hat{x}} - [\hat{K}'(\hat{z}) - \hat{s}]\frac{\partial\hat{\mathcal{G}}}{\partial\hat{z}} - \hat{K}(\hat{z})\frac{\partial^2\hat{\mathcal{G}}}{\partial\hat{z}^2} = 0, \quad \hat{x} > 0, \ 0 < \hat{z} < 1,$$
(28)

subject to

$$\hat{\mathcal{G}}(0,\hat{z}) = 1, \qquad 0 < \hat{z} < 1,$$
(29)

and

$$\partial \hat{\mathcal{G}}/\partial \hat{z}\Big]_{\hat{z}=0} = \hat{Q}\hat{\mathcal{G}}(\hat{x},0), \quad \left[\partial \hat{\mathcal{G}}/\partial \hat{z}\right]_{\hat{z}=1} = 0, \qquad \hat{x} > 0.$$
(30)

Finally, the equations governing the moments can be written in the dimensionless form,

$$\hat{K}(\hat{z})\hat{m}_{j}'' + [\hat{K}'(\hat{z}) - \hat{s}]\hat{m}_{j}' = -j\hat{u}(\hat{z})\hat{m}_{j-1}, \qquad 0 < \hat{z} < 1;
\hat{m}_{j}'(0) = \hat{Q}\hat{m}_{j}(0), \qquad \hat{m}_{j}'(1) = 0$$
(31)

for $j = 1, 2, 3, \ldots$, with $\hat{m}_0(\hat{z}) = 1$.

These equations show that the dimensionless survival function and moments of the settlingdistance distribution depend on the same four parameters $(\hat{D}, \hat{M}, \hat{s}, \text{ and } \hat{Q})$ as do the analogous equations for the settling-time distribution. The roles of parameters \hat{s} and \hat{M} are qualitatively the same as their roles in the hitting-distance problem, which were detailed by McNair and Newbold (2001). We therefore focus here on the roles of \hat{z} and the new parameters \hat{Q} and \hat{D} .

4.2.1 Survival and probability density functions

As illustrated in panels A and B of Figure 4, the effect of increasing \hat{Q} on the settling-distance distribution is basically the same as its effect on the settling-time distribution. Thus, for finite \hat{Q} , the settling-distance survival probability is always greater than the corresponding hitting-distance survival probability, but the survival and probability density functions for the settling distance converge to those for the hitting distance as $\hat{Q} \to \infty$. The location of the mode of the settling-distance survival probability density is also relatively insensitive to changes in \hat{Q} , though its height increases with increasing \hat{Q} while the thickness of the upper tail decreases.

The effect of increasing \hat{D} in the settling-distance problem is also similar to its effect in the settling-time problem, as illustrated in panels C and D of Figure 4. Specifically, increasing \hat{D}



Figure 4. Effects of \hat{D} , \hat{Q} , and \hat{z} on the survival function and dimensionless probability density function of the settling distance. Parameter values and curve descriptions in all panels are the same as in the corresponding panels and curves of Figure 2, except that the present examples are distance-based rather than time-based.

tends to reduce the survival probability for all \hat{x} , increase the height of the mode of the probability density, and decrease the thickness of the upper tail, but it has relatively little effect on the location of the mode.

The effects of \hat{z} on the survival and probability density functions of the settling distance are again very similar to its effects on these properties of the settling time. These effects are illustrated in panels E and F of Figure 4. Note that both the survival and probability density functions are fairly insensitive to \hat{z} , except for sufficiently small values (roughly $\hat{z} \leq 0.05$ and $\hat{z} \leq 0.25$, respectively), and that the probability density function always retains a thick upper tail.

4.2.2 Mean and standard deviation

The effects of increasing \hat{Q} or \hat{D} on the mean and standard deviation of the settling distance are also very similar to their effects on these properties of the settling time, as illustrated in Figure 5. Thus, for finite \hat{Q} , the mean settling distance is always greater than the mean hitting distance (for the same \hat{z}) but converges to it as $\hat{Q} \to \infty$ (panel A), while the mean settling distance decreases as \hat{Q} increases (panel B). In addition, the standard deviation of the settling distance is relatively constant over most of the water column but varies sharply near the bed (panel C).

4.3 Application to FPOM in a natural stream

Cushing et al. (1993) report values for the mean current velocity, depth, bed slope, water temperature, and quiescent particle fall velocity for the Smiley Creek FPOM data discussed in the Introduction. Together with tabulated temperature-dependent values for the kinematic viscosity of water, this is nearly all the information required to compute the settling-distance survival functions predicted by the LEM. However, when the vertical current-velocity profile is calculated using the equations we have presented, the predicted mean (vertically averaged) velocity is found to be substantially greater than the observed value. The same problem occurs if we calculate the mean current velocity using standard open-channel-flow equations based on rough-wall turbulence theory (e.g., Eq. (3.43) of Richards, 2004), which address skin resistance but not form resistance. Evidently, sources of resistance to flow not adequately represented in these equations (notably, form resistance due to bed form, channel sinuosity, various types of channel irregularity, etc.) are important in determining current velocity in Smiley Creek.

Since the main purpose of this example is to illustrate how the settling-distance survival function can be predicted rather than to explain the observed mean current velocity, we resolve this difficult problem for the time being by treating bed shear velocity u_* as a calibration parameter and choosing a value that, when used to calculate the vertical profile of velocity, yields a profile whose mean agrees with the observed value. This approach guarantees a match in mean velocity but does not ensure a match in vertical velocity profile u(z), vertical dispersion function K(z), or the distribution $\mathcal{G}(x, z_0)$ of the particle settling distance. Of course, the unknown sources of resistance to flow that are not adequately represented in the original equations may alter u(z) and K(z) — and hence, $\mathcal{G}(x, z_0)$ in a manner not well approximated by simply adjusting u_* , but we cannot address this possibility with available data.

To compute the settling-distance distribution, we also need to know the initial particle elevation z_0 (or more generally, its distribution) and the values of parameters ψ , D, and Q_0 . None of this information is available, so we proceed as follows. Regarding the initial particle elevation, we choose $z_0 = 0.75H$ as a representative value, then assess the robustness of the results to a range of different choices. Regarding ψ and D, we assume that FPOM particles diffuse (due to Brownian motion and eddy diffusion) like a dye tracer, so that values of $\psi = 1$ and $D = 10^{-9}$ m s⁻² are reasonable.



Figure 5. Effects of \hat{D} and \hat{Q} on vertical profiles of the dimensionless mean and standard deviation of the settling distance. Parameter values and curve descriptions in all panels are the same as in the corresponding panels and curves of Figure 3, except that the present examples are distance-based rather than time-based.

Regarding Q_0 , we have no option other than to treat it as a calibration parameter (with u_* fixed) and seek a value that produces an acceptable fit to the empirical FPOM settling-distance survival function. The full list of parameter values used to compute the settling-distance distribution is as follows:

$$\begin{split} H &= 0.34 \text{ m}, \quad \tan(\theta) = 0.0075, \quad \overline{u} = 0.27 \text{ m s}^{-1}, \quad s = 1.3 \times 10^{-3} \text{ m s}^{-1}, \\ D &= 10^{-9} \text{ m}^2 \text{ s}^{-1}, \quad \text{Temp.} = 15^{\circ} \text{ C}, \quad M = 1.14 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}, \\ \psi &= 1, \quad \kappa = 0.4, \quad u_* = 1.58 \times 10^{-2} \text{ m s}^{-1}, \quad Q_0 = 26.5 \text{ m}^{-1}. \end{split}$$

Computed survival functions for both the settling distance and the hitting distance are shown (in dimensional form) in Figure 6, along with the data previously displayed in Figure 1. Settlingdistance survival functions were calculated for several choices of initial elevation z_0 (namely, 0.25*H*, 0.50*H*, 0.75*H*, and 0.95*H*), but the curves are so similar that only the curve for $z_0 = 0.75H$ is shown in the figure. The similarity of these curves indicates that the survival function in this case is fairly robust to initial particle elevation. This robustness breaks down for initial elevations very close to the bed (roughly $z_0 \leq 0.05H$), but this case does not appear relevant to the data of Cushing et al. (1993), since labeled FPOM was injected at the water surface (with an unknown degree of inertial downward mixing) and therefore would not have instantly concentrated near the bed.



Figure 6. Survival functions for suspended fine particulate organic matter (FPOM) in Smiley Creek, Idaho, in July 1990. Data points and dashed curve are the same as in Figure 1 and represent the empirical settling-distance and theoretical hitting-distance survival functions. The solid curve is the theoretical settling-distance survival function predicted by the LEM (see text for parameter values).

Note that, unlike the theoretical survival function for the hitting distance, the theoretical survival function for the settling distance provides a reasonably good description of the data. These results suggest that the LEM with probabilistic settling is *capable* of accounting for the FPOM data of Cushing et al. (1993), and that particles typically fail to settle on their first encounter with the bottom. A more rigorous test of the model will require a method for obtaining independent estimates of Q_0 (some possible approaches are discussed in the next section), as well as the collection of new data that include accurate characterization of initial particle elevation and sufficient information about vertical mixing (e.g., from a dye study) so that any required adjustment of the equations governing u(z) and K(z) can be made.

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