First Passage Times and Breakthrough Curves Associated with Interfacial Phenomena

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The topic addressed in this paper was initially motivated by questions resulting from recent laboratory experiments designed to empirically test and understand advection-dispersion in the presence of sharp interfaces; e.g., experiments by [6], [5] [4]. Such laboratory experiments have been rather sophisticated in the use of layers of sands and/or glass beads of different granularities and modern measurement technology. As a result they have uncovered a convincing empirical foundation for some interesting and unexpected phenomena that had escaped prior theoretical notice and explanation. To this end it is natural to inquire about the effect of an interface on the stochastic particle motion of immersed solutes. From a general mathematical point of view an *interface* is defined by a hypersurface across which the dispersion coefficient is discontinuous. As is well-known for the case of dilute suspensions in a homogeneous medium (e.g., water), perhaps flowing at a rate v, the particle motion is that of a Brownian motion with a constant diffusion coefficient $D > 0$ and drift v. For simple one-dimensional flow across an interface, a localized point interface results in a skewness effect that explains much of the empirically observed results noted above; see [9], [10], [1], [2], [11].

Problem As an illustration of empirical findings, suppose that a dilute solute is injected at a point L units to the left of an interface at the origin and retrieved at a point L units to the right of the interface. Let D^- denote the (constant) dispersion coefficient to the left of the origin and D^+ that to the right, with say $D^- < D^+$. Conversely, suppose the solute is injected at a point L units to the right of the interface and retrieved at a point L units to the left. *Which will be retrieved first ?*

For positive parameters D^+, D^-, consider a piecewise constant dispersion coefficient with interface at $x = 0$ given by

$$D(x) = D^- 1_{(-\infty,0)}(x) + D^+ 1_{[0,\infty)}(x), \quad x \in \mathbf{R}.$$

Theorem 1 Let D^+, D^- be arbitrary positive numbers, with say $D^- < D^+$. Define $Y_t^{(\alpha^*)} = s(B_t^{(\alpha^*)}), t \geq 0$, where $B^{(\alpha^*)}$ is skew Brownian motion with transmission parameter $\alpha^* = \frac{D^+}{D^+ + D^-}$, and $s(x) = \sqrt{D^+} x 1_{[0,\infty)}(x) + \sqrt{D^-} x 1_{(-\infty,0]}(x), x \in \mathbf{R}$. Let $T_y = \inf\{t \geq 0 : Y_t^{(\alpha^*)} = y\}$. Then,

(a) For smooth initial data c_0, $c(t, y) = E_y c_0(Y_t^{(\alpha)}), \quad t \geq 0$, solves

$$\frac{\partial c}{\partial t} = \frac{1}{2} \frac{\partial}{\partial y}(D(y) \frac{\partial c}{\partial y}), \quad D^+ \frac{\partial c(t, 0^+)}{\partial y} = D^- \frac{\partial c(t, 0^-)}{\partial y}.$$

(b) For $y > 0$, $\quad P_{-y}(T_y > t) \leq \frac{\sqrt{D^-}}{\sqrt{D^+}} P_y(T_{-y} > t) < P_y(T_{-y} > t), \quad t \geq 0.$

Remark *This basic result was obtained [2] in terms of first passage times, however the factor $\sqrt{D^-}/\sqrt{D^+}$ was not included in the statement of the result there. Related phenomena and results on dispersion in this context are also given in [9], [10], [1], [11]. In addition, a formula for the first passage time distribution for skew Brownian motion was recently obtained in [3]. In principle, the identification of stochastic particle motions can have computational advantages. Results pertaining to Monte-Carlo simulations of skew diffusions are described in [7] and references therein.*

As illustrated by the examples below, the role of interfacial phenomena is of much broader interest than suggested by advection-dispersion experiments. However the specific nature of the interface can vary, depending on the specific phenomena. We briefly describe three distinct classes of examples of phenomena from the biological/ecological sciences in which interfaces naturally occur.

Example 1 (**Coastal Upwelling and Fisheries**) Up-wellings, the movement of deep nutrient rich waters to the sun-lit ocean surface, occur in roughly one percent of the ocean but are responsible for nearly fifty-percent of the worlds fishing industry. The up-welling along the Malvinas current that occurs off of the coast of Argentina is unusual in that it is the result of a very sharp break in the shelf, rather than being driven by winds. The equation for the free surface η as a function of spatial variables (x, y) is of the form

$$\frac{\partial \eta}{\partial y} = -\frac{r}{f} \left(\frac{\partial h}{\partial x} \right)^{-1} \frac{\partial^2 \eta}{\partial x^2},$$

where $r > 0$ and $f < 0$ in the southern hemisphere, and $h(x)$ is the depth of the ocean at a distance x from the shore. In particular, the sharp break in the shelf makes $h'(x)$ a piecewise constant function with positive values H^+, H^-. The location of the interface coincides with the distance to the shelf-break. If the spatial variable $y > 0$ is viewed as a "time"parameter, then this is a skew-diffusion equation, however the physics imply continuity of the derivatives $\partial \eta / \partial y$ at the interface; see [8] and references therein.

Example 2 (**Fender's Blue Butterfly**) The Fenders Blue is an endangered species of butterfly found in the pacific northwestern United States. The primary habitat patch is Kinkaid's Lupin flower. Quoting [14], *"Given past research on the Fender's blue, and the potential to investigate response to patch boundaries, we ask two central questions. First, how do organisms respond to habitat edges? Second, what are the implications of this behavior for residence times?"* Sufficiently long residence (occupation) times in Lupin patches are required for pollination, eggs, larvae and ultimate sustainability of the population. Empirical evidence points to a skewness in random walk models for butterfly movement at the path boundaries.

Example 3 (**Sustainability on a River Network**) The movement of larvae in a river system is often modeled by advective-dispersion equations in which the rates are determined by hydrologic/geomorphologic relationships in the form of the so-called *Horton laws.* In general river networks are modeled as directed binary tree graphs and each junction may be viewed as an interface. Conservation of mass leads to continuity of flux of larvae across each stream junction as the appropriate interface condition. Problems on sustainability in this context are generally formulated in terms of network size and characteristics relative to the production of larvae sufficient to prevent permanent downstream removal at low population sizes; see [12] for recent results in the case of a river network.

The following theorem provides a useful summary of the interplay between diffusion coefficients and broader classes of possible interfacial conditions illustrated by these examples. The proof follows by a straightforward application of the Itô-Tanaka formula.

Theorem 2 Let D^+, D^- be arbitrary positive numbers and let $0 < \alpha, \lambda < 1$. Define $Y_t^{(\alpha)} = s(B_t^{(\alpha)}), t \geq 0$, where $B^{(\alpha)}$ is skew Brownian motion with transmission parameter α and $s(x) = \sqrt{D^+}x1_{[0,\infty)}(x) + \sqrt{D^-}x1_{(-\infty,0]}(x),\ x \in \mathbf{R}$. Then

$$M_t = f(Y_t^{(\alpha)}) - \frac{1}{2}\int_0^t D(Y_u^{(\alpha)})f''(Y_u)du, \quad t \geq 0,$$

is a martingale for all $f \in \mathcal{D}_\lambda = \{f \in C^2(\mathbf{R}\backslash\{0\}) \cap C(\mathbf{R}) : \lambda f'(0^+) = (1-\lambda)f'(0^-)\}$ if and only if

$$\alpha = \alpha^*(\lambda) = \frac{\lambda\sqrt{D^-}}{\lambda\sqrt{D^-} + (1-\lambda)\sqrt{D^+}}.$$

Remark *This theorem is a generalization of the results obtained by [9] and [1] for the case of advection-dispersion problems across an interface described at the outset, where the parameter* $\lambda = \frac{D^+}{D^+ + D^-}$ *and* $\alpha^* = \frac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}$.

Definition With the choice of $\alpha^* \equiv \alpha^*(\lambda)$ given by Theorem 2, we refer to the process Y^{α^*} as the *physical diffusion* corresponding to the dispersion coefficients D^+, D^- and interface parameter λ.

Observe that in the application to the coastal up-welling problem one obtains

$$\alpha^* = \frac{\sqrt{D^-}}{\sqrt{D^+} + \sqrt{D^-}}.$$

The physical diffusion for this example may be checked to coincide with the Stoock-Varadahn martingale in this case; see [15] for the definition of the corresponding martingale problem. Note that the answer to the first passage time problem will be exactly opposite to that obtained for advection-dispersion experiments under this model.

We conclude with a result to show that the issue raised in Example 2 relating interfacial conditions to residence times is indeed a sensitive problem.

Theorem 3 Let Y^{α^*} denote the physical diffusion for the dispersion coefficients D^+, D^- and interface parameter λ. Define modified occupation time processes by

$$\tilde{\Gamma}^+(t) = \int_0^t 1[Y_s^{(\alpha^*)} > 0]ds, \quad t \geq 0.$$

Similarly let $\tilde{\Gamma}^-(t) = t - \tilde{\Gamma}^+(t), t \geq 0$. Then,

$$\tilde{\Gamma}^+(t) > \tilde{\Gamma}^-(t) \ \forall t > 0 \quad \Longleftrightarrow \lambda > \frac{\sqrt{D^+}}{\sqrt{D^+} + \sqrt{D^-}},$$

with equality when $\lambda = \frac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}$.

Proof Let $\lambda(x) = 2\lambda 1_{[0,\infty)}(x) + 2(1-\lambda)1_{(-\infty,0)}(x)$, and define $\rho(x) = D(x)/\lambda(x)$. Consider the time change $\tau_\rho(t,\omega)$ defined by

$$\int_0^{\tau_\rho(t)} \frac{1}{\rho(B_s)} = t, \quad t \geq 0.$$

Define S_ρ by $B(t, S_\rho(\omega)) = B(\tau_\rho(t,\omega),\omega) = Z(t,\omega)$. Then the process Z is a diffusion with zero drift and diffusion coefficient $\frac{D^\pm}{\lambda^2(x)}$ with interface parameter $\lambda = 1/2$. Now observe that

$$\begin{aligned}
\Gamma^+_{Y^{(\alpha^*)}}(t) &:= \int_0^t 1[Y_s^{(\alpha^*)} > 0] d < Y^{(\alpha^*)} >_s \\
&= \int_0^t 1[Z_s > 0] 4\lambda^2 d < Z >_s \\
&= 4\lambda^2 \int_0^t 1[B(\tau_\rho(s) > 0] \frac{D^+}{4\lambda^2} ds \\
&= 4\lambda^2 \Gamma_B^+(\tau_\rho(t)).
\end{aligned}$$

Similarly $\Gamma^-_{Y^{(\alpha^*)}}(t) = 4(1-\lambda)^2\Gamma_B^-(\tau_\rho(t))$. Thus $(1-\lambda)^2\Gamma^+_{Y^{(\alpha^*)}}(t) = \lambda^2\Gamma^-_{Y^{(\alpha^*)}}(t)$. Now observe that

$$\tilde{\Gamma}^+_{Y^{(\alpha^*)}}(t) = \int_0^t 1[Z_s > 0] ds = \frac{4\lambda^2}{D^+}\Gamma_B^+(\tau_\rho(t)),$$

and similarly for $\tilde{\Gamma}^+_{Y^{(\alpha^*)}}(t)$, to arrive at

$$\frac{D^-}{(1-\lambda)^2}\tilde{\Gamma}^-(t) = \frac{D^+}{\lambda^2}\tilde{\Gamma}^+(t).$$

The assertion now follows.

It is interesting to note that under the mass conservation interface parameter $\lambda = D^+/(D^+ + D^-)$, the particle will reside longer in the region with the faster dispersion rate. While this is to be expected for physical experiments of dispersion in porous media of the type described above, it shows that the conservative interface condition (defined by this choice of λ) is likely not appropriate for models of animal movement !

Remark *A related phenomena in terms of a "modified local time" is described in [2]. The modification, denoted with the ˜, refers to an integration with respect to Lebesgue measure in place of quadratic variation in the usual mathematical definition of local time and quadratic variation; e.g., see [13]. In general, the treatment of dispersion in the presence of interfaces suggests that the physical/biological theories are, to the extent possible, naturally based on a modification of local times and occupation times in which integration with respect to quadratic variation is replaced by integration with respect to Lebesgue measure. In fact it is shown in [2] that this naturally leads to a stochastic determination of the physical transmission parameter* α^* *in terms of a continuity condition on the modified local time of the stochastic particle motion. This is a probabilistic condition at the particle scale that may be viewed as an alternative to the usual macro-scale pde condition of continuity of flux in particle concentrations.*

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ABSTRACT

Advection and dispersion in highly heterogeneous environments involving interfacial discontinuities in the corresponding drift and dispersion rates are described through disparate examples from the physical and biological sciences. A mathematical framework is formulated to address specific empirical phenomena involving first passage time and occupation time functionals observed in relation to the interfacial parameters.