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Thilanka Iresh Arachchi Appuhamillage for the degree of Doctor of Philosophy in Mathematics presented on August 11, 2011.

Title: Skew Diffusion with Drift : A New Class of Stochastic Processes with Applications to Parabolic Equations with Piecewise Smooth Coefficients

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Enrique A. Thomann

This thesis consists of three subsequent parts addressing the applications of stochastic processes to the analysis and solutions of parabolic equations with discontinuous coefficients that are of mathematical interest.

The first two parts consist of three manuscripts, in which we analyze solutions of Fickian convection dispersion equations with discontinuous coefficients and provide mathematical treatment of solute transport across a sharp interface. We assume the dispersion coefficient is a piecewise constant across a plane (interface), the drift is constant and perpendicular to the interface. Also, assume the flux is continuous across the interface (interface condition). The transition probability density function of the underlying stochastic process, called skew diffusion with drift, is given. As an application, we obtain specific results to explain the interesting types of symmetries and asymmetries in the breakthrough curves of a conservative tracer across a sharp interface. Also, to answer an unsolved problem we give the first passage time density formula of skew Brownian motion.

The third part is essentially an extension of the first two parts. In this part we analyze the stochastic processes associated with convection reaction-diffusion equations with discontinuous coefficients. The geometry of the interface and the condition at the interface considered here are more general than in the first two parts.

Skew Diffusion with Drift : A New Class of Stochastic Processes with Applications to Parabolic Equations with Piecewise Smooth Coefficients

by

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APPROVED:

Major Professor, representing Mathematics

Chair of the Department of Mathematics

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I understand that my thesis will become part of the permanent collection of Oregon State University libraries. My signature below authorizes release of my thesis to any reader upon request.

Thilanka Iresh Arachchi Appuhamillage, Author

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CONTRIBUTION OF AUTHORS

The mathematical results presented in Part 2 (except the last section) and in Part 3 were obtained in close collaboration with Professors Enrique Thomann (Mathematics, OSU), Edward Waymire (Mathematics, OSU), Vrushali Bokil (Mathematics, OSU) and Brian Wood (Environmental Engineering, OSU).

The work presented in last section of Part 2 was obtain in close collaboration with Daniel Sheldon (postdoctoral scholar in Computer Science, OSU).

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1 INTRODUCTION

Discovery of the connection between stochastic processes and parabolic differential equations goes back to the early twentieth century. Connecting the observation of Robert Brown's "Brownian molecular motion" (Brown (1828)), Einstein (1905) showed that if these individual solute molecules in a liquid move independently, and the rate change of their mean-square displacements is constant, say D, then the concentration of solute molecules at time t at the position x, say $c(t, x)$, must obey the diffusion equation,

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}. \tag{1.1}$$

Later with the work of Bachelier (1900, 1912), Smoluchowski (1906) and Wiener (1923), this "Brownian molecular motion" was described as a random process in continuous time (the well known Brownian motion).

In Kolmogorov (1931), he generalized the Markov property to processes in continuous time and showed that the transition probabilities of such Markov processes satisfy the Fokker-Planck equation. This, as well as other work of Kolmogorov (Kolmogorov (1933)), established the connection between parabolic differential equation and the certain type of stochastic processes called Markov processes.

Solutions of stochastic differential equations (SDE) are Markov processes. An important aspect of this Markov processes is that they uniquely determine their transition probabilities. The important connection between such SDEs and the Kolmogorov backward partial differential equation can be proved using the famous Itô's formula which represent diffusions via integrals with respect to Brownian paths and, the Chapmen-Kolmogorov equation.

Much of the theory on stochastic processes and partial differential equations (PDEs) has been developed since the seminal work of Kolmogorov. We would like to mention the work of W. Feller in the classification of one-dimensional diffusions, P. Levy's characterization of Brownian motion, and the work of Itô and McKean (1963) on constructing certain stochastic processes associated with Feller's classification of one-dimensional diffusions in terms of second order differential operators. More recent work includes, the work of Stroock and Varadhan (1979) relating continuous time martingales and differential operators, and the probabilistic reformulation via the Feymann-Kac formula of basic problems in potential theory.

When describing the motion of a small particle suspended in a moving liquid subject to random molecular bombardments, a reasonable mathematical model for the position X_t of the particle at time t would be a stochastic differential equation of the form

$$dX_t = \sigma(t, X_t)dB_t + b(t, X_t)dt \tag{1.2}$$

where b is the velocity of the fluid (called drift vector), B Brownian motion and σ is a square matrix ($\sigma\sigma^T$ called the diffusion matrix). Thus the solution to this SDE, X_t, may be thought of as the mathematical description of the motion of a small particle in a moving fluid and so X_t is called a diffusion process.

The theory of diffusion processes, drawing inspiration from physics, having deep connections with the theory of partial differential equations, and serving as models (or approximations) in diverse fields like ecology, hydrology, engineering, economics (finance), has been an outstanding success of probabilistic methodology, and has in turn played a key role in shaping developments in probability theory.

In this thesis, we study the stochastic processes associated with partial differential equations mostly arising from physical phenomena. All the PDE's studied in this thesis are evolution equations of the form

$$\frac{\partial u}{\partial t} = \mathcal{L}u, \quad t \geq 0, \quad u(0, x) = u_0 \tag{1.3}$$

for u in an appropriate functions space $\mathcal{O}$ and $\mathcal{L}$ is an elliptic operator acting on functions in $\mathcal{O}$. A stochastic process with the state space S and the index set Λ, is a sequence of random variables $X = \{X_r : r \in \Lambda\}$ defined on the same probability space $\{\Omega, \mathcal{F}, \mathbb{P}\}$. Throughout this thesis we consider $S = \mathbb{R}^n$ and $\Lambda = [0, \infty)$. Also when we say that the process X is "associated" with the problem (1.3), it means that for a large class of initial data u_0, the solution to (1.3) is given by

$$u(t, x) = \mathbb{E}_x u_0(X_t), \quad 0 \leq t < T, \tag{1.4}$$

for some $T > 0$, where $\mathbb{E}_x$ denotes expectation with respect to the measure $\mathbb{P}$ such that $\mathbb{P}(X_0 = x) = 1$, and the equality is defined in the sense of functions in $\mathcal{O}$.

In this thesis, we study equations of the type (1.3) with the operator $\mathcal{L}$ having discontinuous coefficient across finitely many hypersurfaces (called interfaces). At these hypersurfaces (interfaces), physical consideration required the functions in $\mathcal{O}$ satisfy an interface condition. In most instances the condition we consider is continuity of flux across the interface. In the final chapter we consider the following more general interface condition

$$\lambda \nabla u \cdot \eta|_+ = (1 - \lambda) \nabla u \cdot \eta|_- \tag{1.5}$$

where η is a unit normal to the interface, $0 \leq \lambda \leq 1$ and $\pm$ represent the two regions separated by the interface. Due to this interface condition, the domain $\mathcal{O}$ of the differential operator does not contain C^2 functions.

The organization of this thesis and brief outline of the problems considered in subsequent chapters are as follows:

This thesis is written in the “manuscript document format” as specified by the Oregon State University Thesis Guide 2006-2007. Each of the three subsequent parts contains manuscripts on the applications of stochastic processes to the analysis and solutions of parabolic equations with discontinuous coefficients. The publication status of each manuscript is specified in the respective part heading page. In the last part of this dissertation the reader can find some concluding remarks, afterthoughts and open problems that did not make it into the submitted manuscripts.

The first part consists of two manuscripts. In the first manuscript we analyze the dispersion equation with piecewise constant dispersion coefficient across a plane (interface) and a constant drift perpendicular to the interface. In addition, we assume the flux is continuous across the interface (interface condition). We compute the transition probability density function of the underlying stochastic process which we refer to as “skew diffusion with drift”. A determination of the (joint) distributions of key functionals of standard skew Brownian motion together with some associated probabilistic semigroup and local time theory is given for these purposes. We also give an important stochastic ordering of first passage times of skew diffusion. At the end of the manuscript we include a section (second manuscript), that computes the formula for the first passage time of skew Brownian motion, which answers an important unsolved problem.

The second part consists of a manuscript that provide a mathematical treatment of solute transport when the mean velocity is perpendicular to a sharp interface. For this case, the resident and flux-averaged concentrations can be derived from Fickian laws of convection-dispersion. In a recently reported approach to (deterministic) Fickian convection-dispersion equations it was shown that the concentration field describing solute transport parallel to a sharp interface could be equivalently expressed in terms of the distribution of a particular skew Brownian motion, Ramirez et al. (2008). The manuscript is an extension of this theory to the case of Fickian convection-dispersion for solute transport in the direction of flow orthogonal to a sharp interface. Just as in the case of parallel interface, this is significant in that it leads to an explicit formula for the concentration field, as well as providing some guidance to the further development of particle tracking methods for representing solute transport in discontinuous media. As an application of this theory we obtain specific results to explain the interesting types of symmetries and asymmetries in the breakthrough curves of a conservative tracer across a sharp interface recently reported by Berkowitz et al. (2009). At the end of this manuscript we include a section that explains asymmetry in occupation times of both sides to the interface.

The third part is essentially an extension of the work in part one to more general parabolic equations (convection reaction-diffusion equations) with discontinuous coefficient across interfaces of more general geometries and more general interface condition of the form (1.5). For this PDE, finding the underlying stochastic process is two fold. We first identify the associated SDE. Then we prove the existence of a unique solution of the SDE. The known methods of proving existence and the uniqueness of solutions to a SDE does not apply here as the SDE we have contains an extra term called local time on a surface. We prove this SDE has a unique solution by constructing the solution of SDE.

2 OCCUPATION AND LOCAL TIMES FOR SKEW BROWNIAN MOTION WITH APPLICATIONS TO DISPERSION ACROSS AN INTERFACE

This chapter is based on material from two already published manuscripts and one under review.

In **Section 2.1 through 2.6,** material from the manuscripts

- Occupation and Local Times for Skew Brownian Motion with Applications to Dispersion Across an Interface by T.A. Appuhamillage, V.A. Bokil, E. Thomann, E. Waymire, B.D. Wood that appeared in *Annals of Applied Probability*, Volume 21, Number 1 (2011), 183-214,
- Correction to : Occupation and Local Times for Skew Brownian Motion with Applications to Dispersion Across an Interface by T.A. Appuhamillage, V.A. Bokil, E. Thomann, E. Waymire, B.D.. To appear in *Annals of Applied Probability*, (2011)

is presented. The only changes from the original manuscripts is that the corrections are incorporated in this version.

Section 2.7, consists of the manuscript currently under review:

- First Passage Time of Skew Brownian Motion. T.A. Appuhamillage, Daniel Sheldon. http://arxiv.org/abs/1008.2989v2.

2.1 Introduction

Skew Brownian motion was introduced by Itô and McKean (1963) to construct certain stochastic processes associated with Feller's classification of one-dimensional diffusions in terms of second order differential operators. This spawned further research leading to a number of subsequent foundational probability papers that highlight interesting and sometimes surprising special structure of skew Brownian motion, see, for example, Walsh (1978); Harrison and Shepp (1981); Ouknine (1990); Le Gall (1984); Barlow et al. (1989, 2001); Burdzy and Chen (2001); Ramirez (2011).

Skew Brownian motion has more recently emerged in connection with diverse applications ranging from a variant on the multi-arm bandit problem [Barlow et al. (2000)], mathematical finance [Decamps et al. (2006)], Monte-Carlo simulation schemes [Lejay and Martinez (2006)], and dispersion in heterogeneous media [Freidlin and Sheu (2000); Ramirez et al. (2006); Ramirez et al. (2008)]. The present paper provides new theoretical results for functionals of skew Brownian motion and its associated semi-group theory (pde), together with an application to recently reported laboratory experiments for advection-dispersion across a sharp interface by Berkowitz et al. (2009). A simple version of one of the basic issues in this regard may be posed as follows.

Question: Consider one-dimensional diffusion with two different diffusion coefficients, say $D^- < D^+$, on the left and right half-lines, respectively. Which is more likely to be removed first: a particle injected at -1 and removed at $+1$, or a particle injected at $+1$ and removed at -1 ?

We will see that the answer to this question is fundamentally tied to a corresponding effect of the interface on α-skew Brownian motion, where $\alpha = \alpha^*$ is a function of the diffusion coefficients D^- and D^+ to be determined, together with a delicate balance with its respective diffusive scalings to the left and right of the interface. In view of this basic role of skew Brownian motion, the paper is organized with an initial focus on new properties of skew Brownian motion to be followed by the more specific application to dispersion across an interface. Readers primarily interested in the application may skip from the end of this introductory section to Section 2.5.

To set some notation and basic definitions, let $B = \{B_t : t \geq 0\}$ denote *standard Brownian motion* on a probability space $(\Omega, \mathcal{F}, P)$. Next, let $J_1, J_2, \dots$ denote a fixed enumeration of the excursion intervals of the reflected process $\{|B_t| : t \geq 0\}$. For a given parameter $\alpha \in (0,1)$, let $\{A_m : m = 1, 2, \dots\}$ be an i.i.d. sequence, independent of B, of Bernoulli ± 1 valued random variables also defined on Ω with $P(A_1 = 1) = \alpha$. Define *α-skew Brownian motion* process $B^{(\alpha)} = \{B_t^{(\alpha)} : t \geq 0\}$ by

$$B_t^{(\alpha)} = \sum_{m=1}^{\infty} \mathbf{1}_{J_m}(t) A_m |B_t|, \tag{2.1}$$

where $\mathbf{1}_S$ denotes the indicator function of the set S. While skew Brownian motion is a continuous semi-martingale, Walsh (1978) showed that its local time is discontinuous. We note that throughout the paper the cases $\alpha = 0$, and $\alpha = 1$ are excluded for simplicity of presentation. All the results in the paper are stated for $0 < \alpha < 1$, with obvious extensions to these other values of the parameter α.

Although the excursion representation (2.1) does not extend to define a "skew Brownian motion with drift", a number of natural alternatives are available.[1] We mention two. The first describes the fundamental process intrinsic to the application to dispersion in porous media from the perspective of semi-group theory. The second is an equivalent formulation from the perspective of martingale theory. In preparation for these descriptions and through the paper, we denote by $\mathbb{R}_0 = (-\infty, 0) \cup (0, \infty) = \mathbb{R} \backslash \{0\}$.

Definition 2.1.1. *For $0 < \alpha < 1, v \in (-\infty, \infty)$, the $\alpha-$skew Brownian motion with drift v $B^{(\alpha,v)}$ is the Markov process with continuous sample paths determined by the infinitesimal*

[1] To the best of our knowledge this process has not been previously named in the literature. However this terminology is consistent with the usual nomenclature associated with the infinitesimal generator.

generator $\frac{1}{2}\frac{d^2}{dx^2}+v\frac{d}{dx}$ *with domain* $\mathcal{D}_{\alpha,0}=\{u\in C^2(\mathbb{R}_0)\cap C(\mathbb{R}):\alpha u'(0^+)=(1-\alpha)u'(0^-)\}$.

The existence of unique strong solutions to stochastic differential equations of the form

$$dY_t=(2\alpha-1)dL_t^Y(0)+v\,dt+\,dB_t, \tag{2.2}$$

where $B=\{B_t:t\geq 0\}$ is standard Brownian motion, and $L_t^Y(0)$ denotes symmetric local time of the process Y at $y=0$, was established by Le Gall (1984). One may also check that the interface condition in Definition 2.1.1 implies that for $f\in\mathcal{D}_{\alpha,0}$

$$M_t=f(Y_t)-\int_0^t\{\frac{1}{2}\frac{d^2}{dx^2}+v\frac{d}{dx}\}f(Y_s)ds,\quad t\geq 0, \tag{2.3}$$

defines a martingale. The following result is generally attributed to Le Gall (1982).

Theorem 2.1.2. *$\alpha-$skew Brownian motion with drift v is the unique strong solution $Y=B^{(\alpha,v)}$ to (2.2).*

In the study of properties of $B^{(\alpha,v)}$, we are naturally led to introduce a process which we denote by ${}^{(\alpha,\gamma)}B$ and refer as *γ-elastic α-skew Brownian motion* (without drift) in analogy to elastic Brownian motion; see, for example, [Itô and McKean (1996), p. 45]. To define this process, let $\gamma>0, 0<\alpha<1$. The process ${}^{(\alpha,\gamma)}B$ is the Markov process with continuous sample paths with infinitesimal generator $\dfrac{1}{2}\dfrac{d^2}{dx^2}$on the domain $\mathcal{D}_{\alpha,\gamma}$, where

$$\mathcal{D}_{\alpha,\gamma}=\{u\in C^2(\mathbb{R}_0)\cap C(\mathbb{R}):\alpha u'(0^+)-(1-\alpha)u'(0^-)=\gamma u(0)\}.$$

The construction of elastic skew Brownian motion defines a process with sample paths in $[\ell_t^{(\alpha)}<R_\gamma]\subset C[0,\infty)$, where R_γ denotes an exponentially distributed random variable with parameter γ, independent of $B^{(\alpha)}$. In particular, the elastic skew Brownian motion agrees with the skew Brownian motion up to the first time $\ell_t^{(\alpha)}>R_\gamma$, after which it is defined to be infinite; see, for example, Itô and McKean (1996) for the case $\alpha=1/2$.

In the next section, we modify techniques of Itô and McKean (1963) to obtain a Feynman–Kac formula for elastic (driftless) skew Brownian motion. Using this, we show that an approach of Karatzas and Shreve (1984) for Brownian motion can be extended to derive the trivariate density of position, symmetric local time at zero, and occupation time of the positive half-line, $(B_t^{(\alpha)}, \ell_t^{(\alpha)}, \Gamma_t^{(\alpha)})$, for (driftless) skew Brownian motion started at zero. Properties of the hitting time at zero for (driftless) skew Brownian motion are then shown to be sufficient to extend this to the trivariate density for the (driftless) skew Brownian motion started at arbitrary $x \in \mathbb{R}$. Some interesting new marginal distributions also follow as corollaries.

Note 2.1.1. *The special notation $\ell_t^{(\alpha)}$ will be reserved to denote the symmetric local time of α-skew Brownian motion at zero throughout this paper. Definitions of left, right, and symmetric local time used here can be found in Revuz and Yor (1991), and will be reviewed in Section 2.5.*

This part of the main results can be more precisely summarized as follows:

Theorem 2.1.3. *Let $l > 0$, and $0 < \tau < t$. Then*

$$P_0\left(B_t^{(\alpha)} \geq y; \ell_t^{(\alpha)} \in dl, \Gamma_t^{(\alpha)} \in d\tau\right) = \begin{cases} \dfrac{2\alpha(1-\alpha)l}{2\pi(t-\tau)^{3/2}\tau^{1/2}} \exp\left\{-\dfrac{((1-\alpha)l)^2}{2(t-\tau)} - \dfrac{(y+\alpha l)^2}{2\tau}\right\} dl d\tau & \textit{if } y \geq 0, \\ \dfrac{2\alpha(1-\alpha)l}{2\pi(t-\tau)^{1/2}\tau^{3/2}} \exp\left\{-\dfrac{(\alpha l)^2}{2\tau} - \dfrac{((1-\alpha)l-y)^2}{2(t-\tau)}\right\} dl d\tau & \textit{if } y \leq 0. \end{cases}$$

The proof of Theorem 2.1.3 is obtained from a Feynman-Kac formula for an elastic skew Brownian motion to obtain a soluble differential equation for the Laplace transform of the trivariate density that may then be inverted; an approach already known from Karatzas and Shreve (1984) to work for standard Brownian motion.

Corollary 2.1.4.

$$P_0\left(B_t^{(\alpha)} \in dy, \ell_t^{(\alpha)} \in dl\right) =$$

$$\begin{cases} \dfrac{2\alpha(l+y)}{\sqrt{2\pi t^3}} \exp\left\{-\dfrac{(l+y)^2}{2t}\right\} dldy & \text{if } y \geq 0, l > 0 \\ \dfrac{2(1-\alpha)(l-y)}{\sqrt{2\pi t^3}} \exp\left\{-\dfrac{(l-y)^2}{2t}\right\} dldy & \text{if } y \leq 0, l > 0 \end{cases}.$$

For an initial state x one has

Corollary 2.1.5. *For $y \geq 0, l > 0, 0 < \tau < t$,*

$$P_x\left(B_t^{(\alpha)} \in dy, \ell_t^{(\alpha)} \in dl, \Gamma_t^{(\alpha)} \in d\tau\right)$$

$$= \begin{cases} \dfrac{\alpha\left[(1-\alpha)l\right]\left[\alpha l + y + x\right]}{\pi(t-\tau)^{3/2}\tau^{3/2}} \exp\left\{-\dfrac{((1-\alpha)l)^2}{2(t-\tau)} - \dfrac{(\alpha l + y + x)^2}{2\tau}\right\} dydld\tau, \text{ if } x \geq 0, \\ \dfrac{\alpha[(1-\alpha)l - x](\alpha l + y)}{\pi(t-\tau)^{3/2}\tau^{3/2}} \exp\left\{-\dfrac{((1-\alpha)l - x)^2}{2(t-\tau)} - \dfrac{(\alpha l + y)^2}{2\tau}\right\} dydld\tau, \text{ if } x \leq 0, \end{cases}$$

whereas for $y \leq 0, l > 0, 0 < \tau < t$,

$$P_x\left(B_t^{(\alpha)} \in dy, \ell_t^{(\alpha)} \in dl, \Gamma_t^{(\alpha)} \in d\tau\right)$$

$$= \begin{cases} \dfrac{(1-\alpha)\left[\alpha l + x\right]\left[(1-\alpha)l - y\right]}{\pi(t-\tau)^{3/2}\tau^{3/2}} \exp\left\{-\dfrac{(\alpha l + x)^2}{2\tau} - \dfrac{((1-\alpha)l - y)^2}{2(t-\tau)}\right\} dydld\tau, \text{ if } x \geq 0, \\ \dfrac{(1-\alpha)\left(\alpha l\right)\left[(1-\alpha)l - y - x\right]}{\pi(t-\tau)^{3/2}\tau^{3/2}} \exp\left\{-\dfrac{(\alpha l)^2}{2\tau} - \dfrac{((1-\alpha)l - y - x)^2}{2(t-\tau)}\right\} dydld\tau, \text{ if } x \leq 0. \end{cases}$$

The following basic corollary identifies the role of the interface of skew Brownian motion in eventually providing an answer to the first passage time question raised at the outset. Define

$$T_y^{(\alpha)} = \inf\{t \geq 0 : B_t^{(\alpha)} = y\}. \tag{2.4}$$

Corollary 2.1.6. *Fix $y \geq 0$. If $1 > \alpha > 1/2$ then*

$$P_{-y}(T_y^{(\alpha)} > t) < P_y(T_{-y}^{(\alpha)} > t), \quad t > 0.$$

Theorem 2.1.7 below establishes a change of measure under which α-skew Brownian motion with drift parameter v is replaced by the elastic (driftless) α-skew Brownian motion with a specific elasticity parameter $\gamma \equiv \gamma(\alpha, v)$. We refer to this as an *elastic change of measure.*

The *elastic change of measure* (via finite-dimensional distributions) is determined on a time interval prior to an elastic explosion as follows. Let

$$\Omega_t = [\ell_t^{(\alpha)} < R_\gamma] \subset C[0, \infty),$$

where R_γ denotes an exponentially distributed random variable with parameter γ, independent of $B^{(\alpha)}$. Then the elastic skew Brownian motion agrees with the skew Brownian motion up to the first time $\ell_t^{(\alpha)} > R_\gamma$. Denote the distributions of $B^{(\alpha,v)}$ and ${}^{(\alpha,\gamma)}B$ on Ω_t by $P_t^{(\alpha,v)}$ and $Q_t^{(\alpha,\gamma)}$, respectively. Also let $p^{(\alpha,v)}(t, x, y)$and $q^{(\alpha,\gamma)}(t, x, y)$ denote their corresponding transition probability densities; note from the elastic construction that $q^{(\alpha,\gamma)}(t, x, y)$ is substochastic.

Theorem 2.1.7. *Fix $t > 0$, and let $\gamma = |(2\alpha - 1)v|$. Then*

$$q^{(\alpha,\gamma)}(t, x, y)dy = \int_0^\infty e^{-\gamma\ell} P_x(B_t^{(\alpha)} \in dy, \ell_t^{(\alpha)} \in d\ell),$$

and

$$p^{(\alpha,v)}(t, x, y) = e^{-v(x-y)-\frac{v^2}{2}t} q^{(\alpha,\gamma)}(t, x, y).$$

In particular, on Ω_t

$$\mathbb{E}_{P_t^{(\alpha,v)}} Y = \mathbb{E}_{Q_t^{(\alpha,\gamma)}} Z_t Y$$

where $Z_t(\omega) = e^{v\omega_t - \frac{v^2}{2}t}$, $\omega \in \Omega_t$.

Remark 2.1.1. *For the case $\alpha = 1/2$, the elastic change of measure exactly coincides with the Cameron-Martin-Girsanov (CMG) transformation for Brownian motion with drift, that is, elastic standard Brownian motion with elasticity $\gamma = 0$ is a standard Brownian motion. However, in view of explosions for elastic diffusions, it is generally much more* *restrictive than CMG. Notice that the elasticity parameter* $\gamma(\alpha, v)$ *specifying the elastic change of measure is invariant under* $\alpha \to 1-\alpha, v \to -v$.

The following formula for the distribution of α-skew Brownian motion with drift v is obtained as a consequence of the elastic change of measure in terms of the tail of the standard normal distribution $\Phi^c(y) = \frac{1}{\sqrt{2\pi}} \int_y^\infty e^{-\frac{z^2}{2}} dz$.

Theorem 2.1.8. *For* $\gamma = |(2\alpha - 1)v|$,

$$P_0(B_t^{(\alpha,v)} \in dy) =$$

$$\begin{cases} \dfrac{2\alpha}{\sqrt{2\pi t}} \exp\Big\{-\dfrac{(y-vt)^2}{2t}\Big\} \Big[1 - \gamma\sqrt{2\pi t}\ \Phi^c\Big(\dfrac{\gamma t + y}{\sqrt{t}}\Big) \exp\Big\{\dfrac{(\gamma t + y)^2}{2t}\Big\}\Big], \\ \text{if } y > 0, \\ \dfrac{2(1-\alpha)}{\sqrt{2\pi t}} \exp\Big\{-\dfrac{(y-vt)^2}{2t}\Big\} \Big[1 - \gamma\sqrt{2\pi t}\ \Phi^c\Big(\dfrac{\gamma t - y}{\sqrt{t}}\Big) \exp\Big\{\dfrac{(\gamma t - y)^2}{2t}\Big\}\Big], \\ \text{if } y < 0. \end{cases}$$

Remark 2.1.2. *A correction in Appuhamillage et al. (2011a) shows the same formula apply for* $\gamma = (2\alpha - 1)v$.

These are the essential preliminary general foundations required for the intended application, but they may also be of independent theoretical value.

The specific application is treated in the last section. First, it involves explicit computation of the concentration curves for particles undergoing dispersion across an interface separating fine and coarse porous media; see Appuhamillage et al. (2010) for plots of resulting concentration curves. The relative notions of *fine* and *coarse* media are defined by their relative dispersion rates $D^- < D^+$; for example, in a saturated fine medium, such as sand, the dispersion of solute concentrations is slower than in a saturated coarse medium, such as large gravel. For the application, we adopt the convention used in experiments in which the fine medium is to the left of the interface and the coarse medium to the right. The injection and retrieval points are located at equal distances from the interface in both fine and coarse, coarse and fine regions, respectively. The flow is oriented in the direction of injection to retrieval points. Second, the application involves an analysis of certain empirically observed symmetries and asymmetries in the concentration curves and breakthrough times, respectively, of dispersion in symmetrically configured fine to coarse and coarse to fine injections and removal arrangements. In answer to the question raised at the outset, it was experimentally observed that fine to coarse breakthrough is faster than coarse to fine breakthrough [Berkowitz et al. (2009)] This has been interpreted as a possible breakdown of basic Fickian flux laws of transport; see Berkowitz et al. (2008). To the contrary, the results of this paper explain the phenomena within the framework of Fickian flux laws. The basic stochastic ordering in Corollary 2.1.6 will be applied to the process of physical dispersion in the final section devoted to the application; that is, the mathematical answer to the question raised at the outset is provided by Corollary 2.5.5.

Finally, the next two results are formulations of individual stochastic particle properties that may serve in place of conservation properties of the concentration in the determination of the transmission parameter α^*. The first is by a variation on the martingale problem. Define the natural scale function by

$$s(x) = \sqrt{D^+}x^+ - \sqrt{D^-}x^-, \quad x \in (-\infty, \infty). \tag{2.5}$$

Martingale Problem (MP): For given $D^\pm$, determine α so that

$$f(s(B_t^{(\alpha)})) - \frac{1}{2}\int_0^t \frac{d}{dy}\left(D(y)\frac{df}{dy}\right)\Big|_{s(B_u^{(\alpha)})} du$$

is a martingale for all $f \in \mathcal{D}_{D^\pm}$ where

$$\mathcal{D}_{D^\pm} = \left\{ g \in C^2(\mathbb{R}_0) \cap C(\mathbb{R}) : D^-\frac{dg}{dy}(0^-) = D^+\frac{dg}{dy}(0^+) \right\}$$

and

$$\frac{d}{dy}\left(D(y)\frac{df}{dy}\right) = \mathbf{1}_{[B_u^{(\alpha)}>0]}D^+\frac{d^2f}{dy^2} + \mathbf{1}_{[B_u^{(\alpha)}\leq 0]}D^-\frac{d^2f}{dy^2}. \tag{2.6}$$

Theorem 2.1.9. *The solution of (MP) for given $D^{\pm}$ is given by the process $Y = s(B^{(\alpha)})$ corresponding to the transmission parameter*

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

Alternatively, α^* can be characterized as the parameter that makes a modification of local time continuous for the skew diffusion. To be precise, for a given stochastic process $Y = \{Y_t : t \geq 0\}$, define right or left *modified local time at a*, respectively, by

$$\tilde{A}_+^Y(t, a) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^t \mathbf{1}([a \leq Y_s < a + \varepsilon]) ds \tag{2.7}$$

and

$$\tilde{A}_-^Y(t, a) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^t \mathbf{1}([a - \varepsilon < Y_s < a]) ds \tag{2.8}$$

As usual, define the symmetric local time by

$$\tilde{A}^Y = \frac{\tilde{A}_-^Y + \tilde{A}_+^Y}{2}. \tag{2.9}$$

The modification (2.7), (2.8),(2.9) to the customary definitions of one-sided and symmetric local times is that the integration is with respect to ds and not with respect to the quadratic variation of Y. However, for the case of $Y = B^{(\alpha)}$, the modified local time coincides with usual local time. A mathematical perspective on Theorem 2.1.10, below, can be obtained by combining the theorem of Walsh (1978) with the celebrated theorem of Trotter (1958) for the determination of the value of α for which this local time is continuous, that is, this yields $\alpha = 1/2$. For the present paper, the extension is motivated by the physical problem as explained in the following Remark 2.1.3 in connection with the application.

Remark 2.1.3. *One may notice that the units of local time coincide with the units of the process, namely length (L) in the case of applications of the type considered here. As a time unit this is interpreted probabilistically as the natural time scale of the diffusion. The units* *of the modified local time (T/L) turn out to be more appropriate for the continuity issue expressed by the following theorem and generalizing Walsh (1978). In general, the reason to consider alternative probabilistic determinations of α^* lies in their potential utility for extensions of the geometry to more complicated interfaces.*

Theorem 2.1.10. *Let $Y_t = s(B_t^{(\alpha)})$. Then the process $\tilde{A}^Y$ is a.s. (spatially) continuous in a iff $\alpha = \alpha^*$.*

2.2 Elastic Skew Brownian Motion and a Feynman–Kac Formula

Fix parameters $\alpha \in (0,1)$ and $\gamma \geq 0$. A probability model for elastic skew Brownian motion may be defined as follows. Let R_γ be an exponentially distributed random variable with parameter $\gamma > 0$ on a probability space $(\Omega', \mathcal{F}', P')$. Define a new process $\{^{(\alpha,\gamma)}B_t : t \geq 0\}$ as the skew Brownian motion $B_t^{(\alpha)}$ "killed"when its local time at zero exceeds the level R_γ. More preciesly, on enlarged probability space $(\widetilde{\Omega}, \widetilde{\mathcal{F}}, \widetilde{P}) = (\Omega \times \Omega', \mathcal{F} \otimes \mathcal{F}', P \times P')$, define $\zeta_\gamma = \inf\{t \geq 0 : \ell_t^{(\alpha)} > R_\gamma\}$. Then we have $\widetilde{P}(\zeta_\gamma > t \mid R_\gamma) = e^{-\gamma \ell_t^{(\alpha)}}$ and the *elastic skew Brownian motion with lifetime* ζ_γ is defined by

$$^{(\alpha,\gamma)}B_t = \begin{cases} B_t^{(\alpha)} & \text{if } t < \zeta_\gamma \\ \infty & \text{if } t \geq \zeta_\gamma. \end{cases} \tag{2.10}$$

In the case $\gamma = 0$, one obtains skew Brownian motion. The transition probability densities $p^{(\alpha)}(t,x,y)$for skew Brownian motion were computed in Walsh (1978) using judicious applications of the reflection principle for Brownian motion. We record the result here for ease of reference

$$p^{(\alpha)}(t,x,y) = \begin{cases} \frac{1}{\sqrt{2\pi t}}e^{-\frac{(y-x)^2}{2t}} + \frac{(2\alpha-1)}{\sqrt{2\pi t}}e^{-\frac{(y+x)^2}{2t}} & \text{if } x>0, y>0 \\ \frac{1}{\sqrt{2\pi t}}e^{-\frac{(y-x)^2}{2t}} - \frac{(2\alpha-1)}{\sqrt{2\pi t}}e^{-\frac{(y+x)^2}{2t}} & \text{if } x<0, y<0 \\ \frac{2\alpha}{\sqrt{2\pi t}}e^{-\frac{(y-x)^2}{2t}} \quad \text{if } x \le 0, y>0 \\ \frac{2(1-\alpha)}{\sqrt{2\pi t}}e^{-\frac{(y-x)^2}{2t}} \quad \text{if } x \ge 0, y<0. \end{cases} \tag{2.11}$$

Next, we obtain a Feynman–Kac formula for this process. To simplify the presentation, let $g(x,t) = \frac{1}{\sqrt{2\pi t}}e^{-\frac{x^2}{2t}}$, and let $h(s;x) = \frac{|x|}{\sqrt{2\pi}}s^{-\frac{3}{2}}e^{-\frac{x^2}{2s}}$; as is very well-known $h(t,x)$ is the first passage time density to zero of standard Brownian motion starting at x, see, for example, [Bhattacharya and Waymire (2009), p. 30]. Note that, by definition in terms of excursions, this coincides with the first passage time to zero for any skew Brownian motion started at x as well. We also recall the following Laplace transforms;

$$\int_0^\infty e^{-\beta t}g(x,t)dt = \frac{1}{\sqrt{2\beta}}\exp\left(-|x|\sqrt{2\beta}\right), \tag{2.12}$$

$$\int_0^\infty e^{-\lambda t}h(x,t)dt = \exp\left(-|x|\sqrt{2\lambda}\right). \tag{2.13}$$

Theorem 2.2.1. *Let $x \in \mathbb{R}$, $y>0$, and $\lambda>0$. Suppose that f is a bounded continuous function on $\mathbb{R}\backslash\{y\}$. Define a function u by*

$$u(x) = \mathbb{E}_x\int_0^\infty e^{-\lambda t}f({}^{(\alpha,\gamma)}B_t)dt = \mathbb{E}_x\int_0^\infty e^{-\lambda t}e^{-\gamma \ell_t^{(\alpha)}}f(B_t^{(\alpha)})dt.$$

Then u is bounded and continuous on $\mathbb{R}$, C^1 on $\mathbb{R}_0$, C^2 on $\mathbb{R}_0\backslash\{y\}$, and

$$(\lambda - \frac{1}{2}\frac{d^2}{dx^2})u = f, \quad \alpha u'(0^+) - (1-\alpha)u'(0^-) = \gamma u(0).$$

Proof. To simplify notation let $\tau_0 = T^{(\alpha)}_{\cdot,0} \equiv T^{(\frac{1}{2})}_{\cdot,0}$. We first make the claim that for f satisfying the hypothesis of the theorem and $\gamma \ge 0$, one has

$$\mathbb{E}_x\int_{\tau_0}^\infty e^{-\lambda t}e^{-\gamma \ell_t^{(\alpha)}}f(B_t^{(\alpha)})dt = \mathbb{E}_x e^{-\lambda\tau_0}\,\mathbb{E}_0\int_0^\infty e^{-\lambda t}e^{-\gamma\ell_t^{(\alpha)}}f(B_t^{(\alpha)})dt \tag{2.14}$$

Indeed, by a simple change of variables and conditioning on the $\sigma-$field $\mathcal{F}_{\tau_0}$ to use the strong Markov property of $B^{(\alpha)}$, the left hand-side can be written as

$$\begin{aligned}
&\mathbb{E}_x \int_0^\infty e^{-\lambda(t+\tau_0)} e^{-\gamma \ell^{(\alpha)}_{t+\tau_0}} f(B^{(\alpha)}_{t+\tau_0}) dt \\
=\ & \mathbb{E}_x \left[\mathbb{E}_x \left[e^{-\lambda \tau_0} \int_0^\infty e^{-\lambda t} e^{-\gamma \ell^{(\alpha)}_{t+\tau_0}} f(B^{(\alpha)}_{t+\tau_0}) dt |\ \mathcal{F}_{\tau_0} \right]\right] \\
=\ & \mathbb{E}_x e^{-\lambda\tau_0}\ \mathbb{E}_0 \int_0^\infty e^{-\lambda t} e^{-\gamma \ell^{(\alpha)}_t} f(B^{(\alpha)}_t) dt
\end{aligned}$$

as claimed.

Then, from the definition of u, noting that $l^{(\alpha)}_t = 0$ for $t < \tau_0$, and using (2.14), one has

$$\begin{aligned}
u(x) &= \mathbb{E}_x \int_0^{\tau_0} e^{-\lambda t} f(B^{(\alpha)}_t) dt + \mathbb{E}_x \int_{\tau_0}^\infty e^{-\lambda t} e^{-\gamma \ell^{(\alpha)}_t} f(B^{(\alpha)}_t) dt \\
&= \mathbb{E}_x \int_0^{\tau_0} e^{-\lambda t} f(B^{(\alpha)}_t) dt + \mathbb{E}_x e^{-\lambda\tau_0}\ \mathbb{E}_0 \int_0^\infty e^{-\lambda t} e^{-\gamma \ell^{(\alpha)}_t} f(B^{(\alpha)}_t) dt \\
&= \mathbb{E}_x \int_0^\infty e^{-\lambda t} f(B^{(\alpha)}_t) dt - \mathbb{E}_x \int_{\tau_0}^\infty e^{-\lambda t} f(B^{(\alpha)}_t) dt + u(0)\mathbb{E}_x e^{-\lambda\tau_0} \\
&= \mathbb{E}_x \int_0^\infty e^{-\lambda t} f(B^{(\alpha)}_t) dt \\
&\quad + \mathbb{E}_x e^{-\lambda\tau_0} \left[u(0) - \mathbb{E}_0 \int_0^\infty e^{-\lambda t} f(B^{(\alpha)}_t) dt \right]
\end{aligned}$$

where in the last step we used (2.14) with $\gamma = 0$.

Therefore, recalling $\mathbb{E}_x e^{-\lambda\tau_0} = e^{-\sqrt{2\lambda}|x|}$, and denoting the Laplace transform of $t \to p^{(\alpha)}(t,x,y)$ for fixed x, y by $\widehat{p}^{(\alpha)}(\lambda, x, y)$, one has

$$u(x) = \int_{-\infty}^\infty \widehat{p}^{(\alpha)}(\lambda,x,y) f(y) dy + e^{-\sqrt{2\lambda}|x|} \left\{ u(0) - \int_{-\infty}^\infty \widehat{p}^{(\alpha)}(\lambda,0,y) f(y) dy \right\}.$$

From (2.11) and (2.13), one has

$$\hat{p}^{(\alpha)}(\lambda,0,y) = \begin{cases} \frac{2\alpha}{\sqrt{2\lambda}} e^{-|y|\sqrt{2\lambda}} & \text{for } y > 0, \\ \frac{2(1-\alpha)}{\sqrt{2\lambda}} e^{-|y|\sqrt{2\lambda}} & \text{for } y < 0. \end{cases} \tag{2.15}$$

In particular, it follows that $\lambda u - \frac{1}{2} u'' = f$ and

$$-\left\{ \alpha u'(0^+) - (1-\alpha) u'(0^-) \right\} + \sqrt{2\lambda} \int_{-\infty}^\infty \widehat{p}^{(\alpha)}(\lambda,0,y) f(y) dy = \sqrt{2\lambda} u(0). \tag{2.16}$$

On the other hand, using the excursion definition of skew Brownian motion

$$
\begin{aligned}
u(0) &= \mathbb{E}_0 \int_0^\infty e^{-\lambda t} e^{-\gamma \ell_t^{(\alpha)}} f(B_t^{(\alpha)}) dt \\
&= \mathbb{E}_0 \int_0^\infty e^{-\lambda t} e^{-\gamma \ell_t^{(\alpha)}} \left[\sum_{n=1}^{\infty} \mathbf{1}_{J_n}(t) f(A_n |B_t|) \right] dt \\
&= \alpha \mathbb{E}_0 \int_0^\infty e^{-\lambda t} e^{-\gamma \ell_t^{(\alpha)}} \left[\sum_{n=1}^{\infty} \mathbf{1}_{J_n}(t) f(|B_t|) \right] dt \\
&\quad + (1-\alpha) \mathbb{E}_0 \int_0^\infty e^{-\lambda t} e^{-\gamma \ell_t^{(\alpha)}} \left[\sum_{n=1}^{\infty} \mathbf{1}_{J_n}(t) f(-|B_t|) \right] dt \\
&= \alpha \mathbb{E}_0 \int_0^\infty e^{-\lambda t} e^{-\gamma \ell_t^{(\alpha)}} f(|B_t^{(\alpha)}|) dt \\
&\quad + (1-\alpha) \mathbb{E}_0 \int_0^\infty e^{-\lambda t} e^{-\gamma \ell_t^{(\alpha)}} f(-|B_t^{(\alpha)}|) dt.
\end{aligned}
$$

Since the local time at 0 of reflected Brownian motion starting at zero coincides with the local time at 0 of skew Brownian motion with parameter α starting at zero, the last expression can be written in terms of the local time of Brownian motion and reflected Brownian motion to yield

$$
\begin{aligned}
u(0) &= \alpha \mathbb{E}_0 \int_0^\infty e^{-\lambda t} e^{-\gamma \ell_t^{(1/2)}} f(|B_t|) dt \\
&\quad + (1-\alpha) \mathbb{E}_0 \int_0^\infty e^{-\lambda t} e^{-\gamma \ell_t^{(1/2)}} f(-|B_t|) dt.
\end{aligned}
$$

Now, in view of Karatzas and Shreve (1984) [(1.5), p. 820], and after computing the indicated Laplace transform, one has

$$
\begin{aligned}
u(0) &= \frac{\alpha}{\gamma + \sqrt{2\lambda}} 2 \int_0^\infty e^{-y\sqrt{2\lambda}} f(y) dy + \frac{1-\alpha}{\gamma + \sqrt{2\lambda}} 2 \int_0^\infty e^{-y\sqrt{2\lambda}} f(-y) dy \\
&= \frac{\sqrt{2\lambda}}{\gamma + \sqrt{2\lambda}} \int_{-\infty}^\infty \widehat{p}^\alpha(\lambda, 0, y) f(y) dy,
\end{aligned}
$$

where in the last step we used (2.15). Thus, noting (2.16), we have $\alpha u'(0^+) - (1 - \alpha) u'(0^-) = \gamma u(0)$. $\square$

2.3 Trivariate Density for Skew Brownian Motion

Here, we first compute the Laplace transform of the density of the pair $(\ell_t^{(\alpha)}, \Gamma_t^{(\alpha)})$ on the event $\left[B_t^{(\alpha)} \geq y\right]$ for $y > 0$ for the skew Brownian motion starting at 0. Since for $\Gamma_t^{(\alpha)\,-} = t - \Gamma_t^{(\alpha)} = \text{meas}\left\{0 \leq s \leq t : B_s^{(\alpha)} < 0\right\}$, the triples $(-B_t^{(\alpha)}, \ell_t^{(\alpha)}, \Gamma_t^{(\alpha)\,-})$ and $(B_t^{(1-\alpha)}, l_t^{(1-\alpha)}, \Gamma_t^{(1-\alpha)})$ are equivalent in law and $\Gamma_t^{(\alpha)} = t - \Gamma_t^{(1-\alpha)}$, we can easily find the Laplace transform of the density of the pair $(\ell_t^{(\alpha)}, \Gamma_t^{(\alpha)})$ on the event $\left[B_t^{(\alpha)} < y\right]$ for $y < 0$ using the previous case. The following is a direct extension of Karatzas and Shreve (1984) analysis of the case of standard Brownian motion ($\alpha = \frac{1}{2}$) to arbitrary $\alpha \in (0, 1)$.

Lemma 2.3.1. *Let λ, β and γ be positive. Then*

$$\mathbb{E}_0 \int_0^\infty \mathbf{1}_{[y,\infty)}(B_t^{(\alpha)}) \exp\left\{-\lambda t - \beta \Gamma_t^{(\alpha)} - \gamma \ell_t^{(\alpha)}\right\} dt =$$

$$\begin{cases} \dfrac{2\alpha\ \exp\left\{-y\sqrt{2(\lambda+\beta)}\right\}}{\sqrt{2(\lambda+\beta)}\left[\gamma + (1-\alpha)\sqrt{2\lambda} + \alpha\sqrt{2(\lambda+\beta)}\right]} & \textit{if } y > 0, \\ \dfrac{2(1-\alpha)\ \exp\left\{y\sqrt{2(\lambda+\beta)}\right\}}{\sqrt{2(\lambda+\beta)}\left[\gamma + \alpha\sqrt{2\lambda} + (1-\alpha)\sqrt{2(\lambda+\beta)}\right]} & \textit{if } y < 0. \end{cases}$$

Proof. For each $x \in \mathbb{R}$, define

$$u(x) = \mathbb{E}_x \int_0^\infty \mathbf{1}_{[y,\infty)}(B_t^{(\alpha)}) \exp\left(-\lambda t - \beta \Gamma_t^{(\alpha)} - \gamma \ell_t^{(\alpha)}\right) dt$$

According to Theorem 2.2.1, $u \in \mathcal{D}_{\alpha,\gamma}$ and satisfies

$$(\lambda + \beta \mathbf{1}_{[0,\infty)}(x))u(x) = \frac{1}{2}u''(x) + \mathbf{1}_{[y,\infty)}, \quad x \in \mathbb{R} \setminus \{0, y\} \tag{2.17}$$

$$\alpha u'(0^+) - (1-\alpha)u'(0^-) = \gamma u(0) \tag{2.18}$$

Considering the case $y > 0$, u has the form

$$u(x) = \begin{cases} c_1 \exp\left\{x\sqrt{2\lambda}\right\} & \text{if } x \leq 0 \\ c_2 \exp\left\{x\sqrt{2(\lambda+\beta)}\right\} + c_3 \exp\left\{-x\sqrt{2(\lambda+\beta)}\right\} & \text{if } 0 \leq x \leq y \\ c_4 \exp\left\{-(x-y)\sqrt{2(\lambda+\beta)}\right\} + \frac{1}{\lambda+\beta} & \text{if } x \geq y \end{cases}$$

where the constants $c_i, 1 \le i \le 4$, are determined by the above conditions. The lemma follows in the case $y > 0$, from the computation of c_1 using the interface condition in (2.17), (2.18). For $y < 0$, simply use the observation above that the triples $(-B_t^{(\alpha)}, \ell_t^{(\alpha)}, \Gamma_t^{(\alpha)\,-})$ and $(B_t^{(1-\alpha)}, l_t^{(1-\alpha)}, \Gamma_t^{(1-\alpha)})$ have the same distribution. □

The expression in Lemma 2.3.1 is the Laplace transform of the density (if it exists) of the pair $(\ell_t^{(\alpha)}, \Gamma_t^{(\alpha)})$ on the event $\left[B_t^{(\alpha)} \ge y\right]$. As in Karatzas and Shreve (1984), it is also possible to invert the Laplace transform to arrive at the trivariate density asserted in Theorem 2.1.3 in the introduction.

Proof of Theorem 2.1.3 & Corollary 2.1.4: We only consider the case $y > 0$. The case $y < 0$ follows by similar arguments. Using Laplace transforms, it is sufficient to establish

$$\int_0^\infty \int_0^t \int_0^\infty e^{-\lambda t - \beta\tau - \gamma l}\left[\frac{2\alpha(1-\alpha)l}{2\pi(t-\tau)^{3/2}\tau^{1/2}} \mathrm{e}^{\left(-\frac{((1-\alpha)\mathrm{l})^2}{2(\mathrm{t}-\tau)} - \frac{(\mathrm{y}+\alpha \mathrm{l})^2}{2\tau}\right)}\right] dl d\tau dt$$
$$= \frac{2\alpha e^{\left(-y\sqrt{2(\lambda+\beta)}\right)}}{\sqrt{2(\lambda+\beta)}\left[\gamma + (1-\alpha)\sqrt{2\lambda} + \alpha\sqrt{2(\lambda+\beta)}\right]}, \quad y > 0.$$

Reversing the order of integration, and using (2.13) and (2.12), we can write the left-hand side as

$$2\alpha \int_0^\infty e^{-\gamma l} \int_0^\infty e^{-\beta\tau} \int_\tau^\infty e^{-\lambda t} h(t-\tau, (1-\alpha)l)\ dt\ g(\tau, y+\alpha l)\ d\tau\ dl$$
$$= 2\alpha \int_0^\infty e^{-\gamma l} \exp\left(-(1-\alpha)l\sqrt{2\lambda}\right) \int_0^\infty e^{-(\lambda+\beta)\tau}\ g(\tau, y+\alpha l)\ d\tau\ dl$$
$$= 2\alpha \int_0^\infty e^{-\gamma l} \frac{1}{\sqrt{2(\lambda+\beta)}} \exp\left(-(1-\alpha)l\sqrt{2\lambda} - (y+\alpha l)\sqrt{2(\lambda+\beta)}\right) dl$$
$$= \frac{2\alpha e^{\left(-y\sqrt{2(\lambda+\beta)}\right)}}{\sqrt{2(\lambda+\beta)}\left[\gamma + (1-\alpha)\sqrt{2\lambda} + \alpha\sqrt{2(\lambda+\beta)}\right]}$$

□

The trivariate density of position, local time and occupation time of skew Brownian motion, can be obtained by differentiating with respect to y to yield:

$$P_0\left\{B_t^{(\alpha)} \in dy, \ell_t^{(\alpha)} \in dl, \Gamma_t^{(\alpha)} \in d\tau\right\} \tag{2.19}$$
$$= \begin{cases} \dfrac{\alpha\left[(1-\alpha)l\right]\left[\alpha l+y\right]}{\pi(t-\tau)^{3/2}\tau^{3/2}} \exp\left\{-\dfrac{((1-\alpha)l)^2}{2(t-\tau)} - \dfrac{(\alpha l+y)^2}{2\tau}\right\} dydld\tau \\ \qquad \text{if } y>0, l>0, 0<\tau<t, \\ \dfrac{(1-\alpha)\left[\alpha l\right]\left[(1-\alpha)l-y\right]}{\pi(t-\tau)^{3/2}\tau^{3/2}} \exp\left\{-\dfrac{(\alpha l)^2}{2\tau} - \dfrac{((1-\alpha)l-y)^2}{2(t-\tau)}\right\} dydld\tau \\ \qquad \text{if } y<0, l>0, 0<\tau<t. \end{cases}$$

Integrating out τ in (2.19), we obtain the joint distribution of skew Brownian motion with parameter α and its local time at 0 asserted in Corollary 2.1.4.

Integrating out y, l in (2.19) we recover the probability density function of the occupation time for skew Brownian motion with parameter α starting at 0; see Revuz and Yor (1991), and Ramirez et al. (2008) for alternative approaches to this particular case.

Corollary 2.3.2.

$$P_0\left(\Gamma_t^{(\alpha)} \in d\tau\right) = \frac{\alpha(1-\alpha)t}{\pi(t-\tau)^{1/2}\tau^{1/2}\left[(1-\alpha)^2\tau+\alpha^2(t-\tau)\right]} d\tau; \quad 0<\tau<t$$

Integrating out y, τ in (2.19) provides the distribution of local time of skew Brownian motion at zero. As expected, it coincides with that for reflected Brownian motion but is included here as a simple verification.

Corollary 2.3.3.

$$P_0\left(\ell_t^{(\alpha)} \in dl\right) = \frac{2}{\sqrt{2\pi t}} \exp\left\{-\frac{l^2}{2t}\right\} dl, \quad t>0.$$

Proof of Corollary 2.1.5:

The computation of $P_x\left(B_t^{(\alpha)} \in dy, \ell_t^{(\alpha)} \in dl, \Gamma_t^{(\alpha)} \in d\tau\right)$ from Theorem 2.1.3 for $x \neq 0$ will follow from standard convolution properties of first passage time densities at zero of Brownian motion since they coincide with those of skew Brownian motion. Recall that

$h(\cdot;x)$ denotes the first passage time density to zero for (skew) Brownian motion starting at $x > 0$. Then, the strong Markov property for Brownian motion yields

$$h\left(\cdot;x_1+x_2\right)=h\left(\cdot;x_1\right)*h\left(\cdot;x_2\right),\quad x_1x_2>0 \tag{2.20}$$

Thus, for $l > 0, 0 < \tau < t$, we can write the results of (2.19) as,

$$P_0\left(B_t^{(\alpha)}\in dy,\ell_t^{(\alpha)}\in dl,\Gamma_t^{(\alpha)}\in d\tau\right)$$
$$=\begin{cases}2\alpha h\left(t-\tau;(1-\alpha)l\right)h\left(\tau;\alpha l+y\right) & \text{if } y>0,\\ 2(1-\alpha)h\left(\tau;\alpha l\right)h\left(t-\tau;(1-\alpha)l-y\right) & \text{if } y<0.\end{cases}$$

To obtain the trivariate density when $B_0^{(\alpha)} = x$, we use the strong Markov property of skew Brownian motion and the already noted fact that $T_0^{(\alpha)} = T_0^{(1/2)}$ in distribution under P_x, to obtain

$$\begin{aligned}&P_x\left(B_t^{(\alpha)}\in dy,\ell_t^{(\alpha)}\in dl,\Gamma_t^{(\alpha)}\in d\tau\right)\\&=P_x\left(B_t^{(\alpha)}\in dy,\ell_t^{(\alpha)}\in dl,\Gamma_t^{(\alpha)}\in d\tau,T_0^{(\alpha)}\le\tau\right)\\&=\int_{s=0}^{\tau}P_x\left(B_t^{(\alpha)}\in dy,\ell_t^{(\alpha)}\in dl,\Gamma_t^{(\alpha)}\in d\tau|T_0^{(\alpha)}=s\right)P_x\left(T_0^{(1/2)}\in ds\right)\\&=\int_{s=0}^{\tau}P_0\left(B_{t-s}^{(\alpha)}\in dy,l_{t-s}^{(\alpha)}\in dl,\Gamma_{t-s}^{(\alpha)}\in d\tau-s\right)h(s;x)ds.\end{aligned}$$

Considering the case $x \geq 0, y < 0$, and using Theorem (2.1.3) the last expression can be written as

$$\begin{aligned}&=2(1-\alpha)\int_0^{\tau}h\left(\tau-s;\alpha l\right)h\left(t-\tau;(1-\alpha)l-y\right)h\left(s;x\right)dsdydld\tau\\&=2(1-\alpha)h\left(\tau;\alpha l+x\right)h\left(t-\tau;(1-\alpha)l-y\right)dydld\tau,\end{aligned}$$

using the convolution property (2.20).

A similar computation yields that for $x \geq 0,\ y > 0,\ 0 < \tau < t$ and on the event $[T_0^{(\alpha)} < t]$,

$$\begin{aligned}&P_x\left(B_t^{(\alpha)}\in dy,\ell_t^{(\alpha)}\in dl,\Gamma_t^{(\alpha)}\in d\tau,[T_0^{(\alpha)}<t]\right)\\&\qquad=2\alpha h\left(t-\tau;(1-\alpha)l\right)h\left(\tau;\alpha l+y+x\right)dydld\tau.\end{aligned}$$

□

Remark 2.3.1. *We note that if $x \geq 0, y > 0$ one also needs to consider the case that the skew Brownian motion does not reach the origin. In this case, one has*

$$\begin{aligned} & P_x\left(B_t^{(\alpha)} \in dy, \ell_t^{(\alpha)} = 0, \Gamma_t^{(\alpha)} = t\right) \\ = \; & P_x\left(B_t^{(\alpha)} \in dy, T_0^{(\alpha)} \geq t\right) \\ = \; & \frac{1}{\sqrt{2\pi t}}\left[\exp\left\{-\frac{(y-x)^2}{2t}\right\} - \exp\left\{-\frac{(y+x)^2}{2t}\right\}\right] dy;\; x \geq 0,\; y \geq 0. \end{aligned}$$

Corollary 2.3.4. *If $x \geq 0$ we have*

$$P_x(B_t^{(\alpha)} \in dy, \ell_t^{(\alpha)} \in d\ell) =$$
$$\begin{cases} \dfrac{2(1-\alpha)(l-y+x)}{\sqrt{2\pi t^3}} \exp\Big\{ - \dfrac{(l-y+x)^2}{2t}\Big\} dy dl \\ \text{if } \; y \leq 0,\; l \geq 0 \\ \dfrac{2\alpha(l+y+x)}{\sqrt{2\pi t^3}} \exp\Big\{ - \dfrac{(l+y+x)^2}{2t}\Big\} dy dl \\ + \dfrac{1}{\sqrt{2\pi t}}\left[\exp\Big\{-\dfrac{(y-x)^2}{2t}\Big\} - \exp\Big\{-\dfrac{(y+x)^2}{2t}\Big\}\right] \delta_0(dl) dy \\ \text{if } \; y \geq 0,\; l \geq 0, \end{cases}$$

whereas if $x \leq 0$, then

$$P_x(B_t^{(\alpha)} \in dy, \ell_t^{(\alpha)} \in d\ell) =$$
$$\begin{cases} \dfrac{2\alpha(l+y-x)}{\sqrt{2\pi t^3}} \exp\Big\{ - \dfrac{(l+y-x)^2}{2t}\Big\} dy dl \\ \text{if } \; y \geq 0,\; l \geq 0 \\ \dfrac{2(\alpha-1)(l-y-x)}{\sqrt{2\pi t^3}} \exp\Big\{ - \dfrac{(l-y-x)^2}{2t}\Big\} dy dl \\ + \dfrac{1}{\sqrt{2\pi t}}\left[\exp\Big\{-\dfrac{(y-x)^2}{2t}\Big\} - \exp\Big\{-\dfrac{(y+x)^2}{2t}\Big\}\right] \delta_0(dl) dy \\ \text{if } \; y \leq 0,\; l \geq 0 \end{cases}$$

Remark 2.3.2. *Preceding corollary is the corrected corollary appeared in Appuhamillage et al. (2011a).*

While the following formula is relatively more complicated, it is easily computed and plays an essential role in the application given in the next section. For the application, it is sufficient to consider $x < 0, y > 0$, moreover, the other cases may be obtained similarly obtained from the trivariate density.

Corollary 2.3.5. *For $x < 0$ and $y \geq 0$,*

$$\begin{aligned}
&P_x\left(B_t^{(\alpha)} \in dy, \Gamma_t^{(\alpha)} \in d\tau\right) \\
&= \frac{(1-\alpha)}{\pi\sqrt{\tau(t-\tau)}} \frac{(1-\alpha)^3\tau y - \alpha^3(t-\tau)y}{\left[\alpha^2(t-\tau)+(1-\alpha)^2\tau\right]^2} \exp\left(\frac{-\xi(x^2,y^2,\tau,t)}{\xi(\tau,t-\tau,\tau,t)}\right) \\
&\quad + \sqrt{\frac{2}{\pi}} \frac{\alpha(1-\alpha)^2}{\left[\alpha^2(t-\tau)+(1-\alpha)^2\tau\right]^{3/2}} \times \Phi^c\Big(\frac{\sqrt{2}\xi(\alpha x, -(1-\alpha)y, \tau, t)}{\sqrt{\xi(\tau,t-\tau,\tau,t)}}\Big) \\
&\quad \times \big[1 - 2\frac{(\xi(x^2,y^2,\tau,t) - \xi^2(\alpha x, -(1-\alpha)y,\tau,t))}{\xi(\tau,t-\tau,\tau,t)}\big] \\
&\quad \times \exp(-\frac{(\xi(x^2,y^2,\tau,t) - \xi^2(\alpha x, -(1-\alpha)y,\tau,t))}{(\xi(\tau,t-\tau,\tau,t))}),
\end{aligned}$$

where

$$\xi(u,w,\tau,t) = \frac{u(t-\tau)+w\tau}{\alpha^2(t-\tau)+(1-\alpha)^2\tau}.$$

Proof. Let

$$A = \frac{\alpha x(t-\tau) - (1-\alpha)y\tau}{\alpha^2(t-\tau)+(1-\alpha)^2\tau}, B = \frac{\alpha^2(t-\tau)+(1-\alpha)^2\tau}{2\tau(t-\tau)},$$

and

$$C^2 = \frac{x^2(t-\tau)+y^2\tau}{\alpha^2(t-\tau)+(1-\alpha)^2\tau}.$$

For $x \geq 0,\ y > 0,\ \ell > 0,\ 0 < \tau < t$, one has after rather lengthy differentiations

$$
\begin{aligned}
&P_x\left(B_t^{(\alpha)} \in dy, \Gamma_t^{(\alpha)} \in d\tau\right) = \\
&\quad \frac{-2(1-\alpha)}{2\pi\sqrt{\tau(t-\tau)}}\frac{\partial}{\partial x}\frac{\partial}{\partial y}\int_0^\infty \exp\left\{-\frac{(\alpha\ell + x)^2}{2\tau}\right\}\exp\left\{-\frac{((1-\alpha)\ell - y)^2}{2(t-\tau)}\right\}d\ell \\
&\qquad = \frac{(1-\alpha)}{\pi\sqrt{\tau(t-\tau)}}\frac{(1-\alpha)^3\tau x - \alpha^3(t-\tau)y}{\left[\alpha^2(t-\tau) + (1-\alpha)^2\tau\right]^2}\exp(-BC^2) \\
&\qquad + \frac{\alpha(1-\alpha)^2}{\pi\sqrt{\tau(t-\tau)}}\frac{1}{\left[\alpha^2(t-\tau) + (1-\alpha)^2\tau\right]}\frac{\sqrt{\pi}}{\sqrt{B}}\Phi^c(A\sqrt{2B}) \\
&\qquad\qquad \times\left[1 - 2B(C^2 - A^2)\right]\exp(-B(C^2 - A^2)). \quad (2.21)
\end{aligned}
$$

□

2.4 Elastic Change of Measure and Applications to Skew Brownian Motion with Drift

The objective of this section is to establish the elastic change of measure relation between skew Brownian motion with drift and the elastic (driftless) skew Brownian motion defined by Theorem 2.1.7, and apply it to obtain transition probabilities for skew Brownian motion with drift together with the stochastic ordering of passage times.

Proof of Theorem 2.1.7: Recall that α-skew Brownian motion with drift v is denoted by $B^{(\alpha,v)}$ and its transition probability by $p^{(\alpha,v)}(t,x,y)$. Then for $c(t,x) = \mathbb{E}_x c_0(B^{(\alpha,v)}) = \int_{-\infty}^{\infty} c_0(y)p^{(\alpha,v)}(t,x,y)dy$ one has $c \in \mathcal{D}_{\alpha,0}$ and

$$
\begin{gathered}
\frac{\partial c}{\partial t} = \frac{1}{2}\frac{\partial^2 c}{\partial x^2} + v\frac{\partial c}{\partial x} \\
c(t,0^+) = c(t,0^-), \quad \alpha\frac{\partial c}{\partial x}(t,0^+) = (1-\alpha)\frac{\partial c}{\partial x}(t,0^-) \\
c(0,x) = c_0(x).
\end{gathered}
$$

Defining $\tilde{c}(t,x) = \exp\{vx\}c(t,x)$ we obtain

$$\frac{\partial \tilde{c}}{\partial t} = \frac{1}{2}\frac{\partial^2 \tilde{c}}{\partial x^2} - \frac{v^2}{2}\tilde{c}$$

$$\tilde{c}(t,0^+) = \tilde{c}(t,0^-), \quad \alpha\frac{\partial \tilde{c}}{\partial x}(t,0^+) - (1-\alpha)\frac{\partial \tilde{c}}{\partial x}(t,0^-) = (1-2\alpha)v\tilde{c}(t,0)$$

$$\tilde{c}(0,x) = \exp\{vx\}c_0(x)$$

Let $\gamma = |(1-2\alpha)v|$. Then from the Feynman-Kac formula, we have

$$\tilde{c}(t,x) = \mathbb{E}_x \tilde{c}_0({}^{(\alpha,\gamma)}B_t)\exp\Big\{-\frac{v^2}{2}t\Big\} = \int_{-\infty}^{\infty} \tilde{c}_0(y)\exp\Big\{-\frac{v^2}{2}t\Big\}q^{(\alpha,\gamma)}(t,x,y)dy$$

But since $c(t,x) = \exp\{-vx\}\tilde{c}(t,x)$, we have

$$\int_{-\infty}^{\infty} c_0(y)p^{(\alpha,v)}(t,x,y)dy = \int_{-\infty}^{\infty} c_0(y)\exp\Big\{-v(x-y) - \frac{v^2}{2}t\Big\}q^{(\alpha,\gamma)}(t,x,y)dy$$

Thus, the elastic change of measure relation follows as

$$p^{(\alpha,v)}(t,x,y) = \exp\Big\{-v(x-y) - \frac{v^2}{2}t\Big\}q^{(\alpha,\gamma)}(t,x,y).$$

$\square$

Proof of Theorem 2.1.8: Recall that ${}^{(\alpha,\gamma)}B_t$ agrees with $B_t^{(\alpha)}$ when $l_t^{(\alpha)} \leq R_\gamma$. Thus, letting $f^{(\alpha)}(t,x;\cdot,\cdot)$ denote the joint density of $(B_t^{(\alpha)}, \ell_t^{(\alpha)})$ with $B_0^{(\alpha)} = x$,

$$\begin{aligned}
\mathbb{E}_x \tilde{c}_0({}^{(\alpha,\gamma)}B_t) &= \mathbb{E}_x\Big[\tilde{c}_0(B_t^{(\alpha)})\mathbf{1}_{[l_t^{(\alpha)}(B^{(\alpha)})\leq R_\gamma]}\Big] \\
&= \int_0^\infty \mathbb{E}_x\Big[\tilde{c}_0(B_t^{(\alpha)})\mathbf{1}_{[l_t^{(\alpha)}\leq r]}\Big]\gamma\exp\{-\gamma r\}dr \\
&= \int_0^\infty\int_{-\infty}^\infty\int_0^r \tilde{c}_0(y)f^{(\alpha)}(t,x;y,l)\gamma\exp\{-\gamma r\}dldydr \\
&= \int_{-\infty}^\infty\int_0^\infty\int_l^\infty \tilde{c}_0(y)f^{(\alpha)}(t,x;y,l)\gamma\exp\{-\gamma r\}drdldy \\
&= \int_{-\infty}^\infty\int_0^\infty \tilde{c}_0(y)f^{(\alpha)}(t,x;y,l)\exp\{-\gamma l\}dldy.
\end{aligned}$$

Also since

$$\mathbb{E}_x \tilde{c}_0({}^{(\alpha,\gamma)}B_t) = \int_{-\infty}^{\infty} \tilde{c}_0(y)q^{(\alpha,\gamma)}(t,x,y)dy,$$

one has

$$q^{(\alpha,\gamma)}(t,x,y) = \int_0^\infty f^{(\alpha)}(t,x;y,l)\exp\{-\gamma l\}dl. \tag{2.22}$$

From Corollary 2.1.4,

$$f^{(\alpha)}(t,0;y,l) = \begin{cases} \dfrac{2\alpha(l+y)}{\sqrt{2\pi t^3}}\exp\left\{-\dfrac{(l+y)^2}{2t}\right\} & \text{if } y>0, l>0 \\ \\ \dfrac{2(1-\alpha)(l-y)}{\sqrt{2\pi t^3}}\exp\left\{-\dfrac{(l-y)^2}{2t}\right\} & \text{if } y<0, l>0 \end{cases} \tag{2.23}$$

Recognizing from (2.22) that $q^{(\alpha,\gamma)}(t,0,y)$ is the Laplace transform with respect to local time l of $f^{(\alpha)}(t,0,y,l)$, the theorem follows by a direct calculation of this Laplace transform and Theorem 2.1.7. □

Our objective is to next prove the more fundamental stochastic ordering of Corollary 2.1.6 for skew Brownian motion. Although the relevance to the question raised in the Introduction is given in the next section, Corollary 2.1.6 may also be of independent interest apart from the application.

Lemma 2.4.1. *Suppose that $X = X_1 + X_2$ and $Y = Y_1 + Y_2$ are respective sums of independent non-negative random variables. If X_i is stochastically smaller than Y_i, for $i = 1, 2$, then X is stochastically smaller than Y.*

Proof. For $t > 0$,

$$\begin{aligned} P(X>t) &= \int_0^t P(X_1 > t-s)P(X_2 \in ds) \\ &\le \int_0^t P(Y_1 > t-s)P(X_2 \in ds) \\ &= \int_0^t P(X_2 > t-s)P(Y_1 \in ds) \\ &\le \int_0^t P(Y_2 > t-s)P(Y_1 \in ds) \\ &= P(Y>t). \end{aligned} \tag{2.24}$$

□

Proof of Corollary 2.1.6: Let $T_0 \equiv T_0^{(1/2)}$ denote the first time for standard Brownian motion to reach zero. Also note that $T_0^{(\alpha)}$ is distributed as T_0 under P_y for $y \neq 0$, $0 < \alpha < 1$. So clearly for $t \geq 0$, one has

$$P_y(T_0^{(\alpha)} > t) = P_y(T_0 > t) = P_{-y}(T_0 > t) = P_{-y}(T_0^{(\alpha)} > t). \tag{2.25}$$

Now observe, using the strong Markov property of skew Brownian motion,

$$P_{-y}(T_y^{(\alpha)} > t) = \int_0^t P_0(T_y^{(\alpha)} > t - s) P_{-y}(T_0 \in ds), \tag{2.26}$$

and

$$P_y(T_{-y}^{(\alpha)} > t) = \int_0^t P_0(T_y^{(1-\alpha)} > t - s) P_{-y}(T_0 \in ds). \tag{2.27}$$

Next, consider the following coupled representations of the α-*skew Brownian motion* processes $B^{(\alpha)} = \{B_t^{(\alpha)} : t \geq 0\}$: Let $\{U_m : m = 1, 2, \dots\}$ be an i.i.d. sequence, independent of $B^{(\alpha)}$, of uniformly distributed random variables on $[0, 1]$ also defined on Ω by

$$B_t^{(\alpha)} = \sum_{m=1}^{\infty} \mathbf{1}_{J_m}(t)\{2\mathbf{1}_{[0,\alpha)}(U_n) - 1\}|B_t|, \tag{2.28}$$

where $\mathbf{1}_S$ denotes the indicator function of the set S. Then, for any $t > 0$, one has for $1 > \alpha > 1/2$ that

$$[T_y^{(\alpha)} > t] \subset [T_y^{(1-\alpha)} > t].$$

The asserted stochastic ordering follows by application of the lemma to (2.26) and (2.27).

□

2.5 Application to Solute Dispersion Across an Interface

In analogy with the Fourier flux law for heat conduction, the standard model of advection-dispersion is based on Ficks' linear flux law together with continuity of concentration and flux across the interface. For the application treated here, the flux is aligned with the $y-$axis, and the concentration field is uniform in the other two orthogonal directions. Thus, the Fickian (macro-scale) conservation laws can be reduced to an advection-dispersion equation of the form

$$\frac{\partial c}{\partial t} = \frac{1}{2}\frac{\partial}{\partial y}(D(y)\frac{\partial c}{\partial y}) - \frac{\partial vc}{\partial y} \tag{2.29}$$

$$c(t,0^+) = c(t,0^-), \qquad D^+\frac{\partial c}{\partial y}(t,0^+) = D^-\frac{\partial c}{\partial y}(t,0^-), \tag{2.30}$$

where

$$D(y) = \begin{cases} D^- & \text{if} \quad y < 0. \\ D^+ & \text{if} \quad y \geq 0. \end{cases} \tag{2.31}$$

Note 2.5.1. *In treating the application in this paper we have adhered to the standard probability notation of $\frac{1}{2}D$ in place of D in the concentration Equation (2.29).*

In particular, from a probabilistic point of view the particle motion is given by the unique strong solution to

$$dY_t = \frac{D^+ - D^-}{D^+ + D^-}dL_t^0(Y) + v\,dt + \sqrt{D(Y_t)}\,dB_t \tag{2.32}$$

where $B = \{B_t : t \geq 0\}$ is standard Brownian motion. In the case $v = 0$, $Y_t \equiv S_t^*$ is given by

$$S_t^* = s(B_t^{(\alpha^*)}) = \begin{cases} \sqrt{D^+}B_t^{(\alpha^*)} & \text{if} \quad B_t^{(\alpha^*)} \geq 0 \\ \sqrt{D^-}B_t^{(\alpha^*)} & \text{if} \quad B_t^{(\alpha^*)} < 0. \end{cases} \tag{2.33}$$

where $\alpha^* = \frac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}$ and $s(x) = \sqrt{D^+}x^+ - \sqrt{D^-}x^-$ is the natural scale function; see Ramirez (2007). In general, we refer to the process Y given by (2.32) as the *physical skew diffusion with drift* v for the problem (2.29).

Remark 2.5.1. *The advective-dispersive movement of solutes through a porous medium in the presence of a discontinuous interface separating fine and coarse regions is a topic of both active experimental and theoretical interest (Hoteit et al. (2002); LaBolle et al. (1998, 2000); Kuo et al. (1999a), Berkowitz et al. (2009); Ramirez et al. (2006, 2008)).*

The results obtained in Ramirez et al. (2006) for a re-scaling of α-skew Brownian motion for a uniquely determined value of α as the underlying stochastic particle motion governing the (deterministic) Fickian advection-dispersion concentration in the presence of the sharp interface parallel to the flow made it possible to obtain the time-asymptotic central limit theorem and effective dispersion rate, extending the classic Taylor-Aris formula to this setting. This also provided the theoretical foundation for the correct Monte-Carlo approach among those considered in connection with experiments parallel to the flow by Hoteit et al. (2002); see Ramirez et al. (2008). However, the absence of drift in the particle coordinate associated with the α-skew Brownian motion was essential for those developments.

The results of the previous sections now provide an approach to explicitly compute the concentration curves for flow orthogonal to an interface; see Berkowitz et al. (2009). The following bivariate distribution of the position and occupation time is algebraically more complicated than for that of position and local time, for example, Corollary 2.1.4, but it is most relevant to our application in this section.

The transition probabilities of the physical skew dispersion with drift v are obtained in the following theorem. Note that from the definition of S_t^* in (2.33), the occupation time of the positive semiaxis of S^* equals $\Gamma_t^{(\alpha^*)}$, the occupation time by $B_t^{(\alpha^*)}$ of the positive semiaxis. Likewise, the joint density of position and occupation time of S^* and $B^{(\alpha^*)}$ satisfy

$$f_{(S_t^*,\Gamma_t^{(\alpha^*)})}(y;z,\tau) = \frac{1}{\sqrt{D(z)}} f_{(B_t^{(\alpha^*)},\Gamma_t^{(\alpha^*)})}\Big(\frac{y}{\sqrt{D(y)}}; \frac{z}{\sqrt{D(z)}}, \tau\Big), \tag{2.34}$$

where $f_{(B_t^{(\alpha^*)},\Gamma_t^{(\alpha^*)})}$ is given in Corollary 2.3.5.

Theorem 2.5.1. *The transition probability densities for the physical skew diffusion process Y with drift v defined by (2.32) are given by*

$$p(t,y,z) = \mathrm{e}^{\left(\frac{\mathrm{v}}{\mathrm{D(z)}}\mathrm{z} - \frac{\mathrm{v}^2}{2\mathrm{D}^-}\mathrm{t}\right)} \mathrm{e}^{\left(-\frac{\mathrm{v}}{\mathrm{D(y)}}\mathrm{y}\right)} \hat{\mathrm{f}}_{(\mathrm{S}_t^*,\Gamma_t^{(\alpha^*)})}(\mathrm{z};\mathrm{y},\frac{\mathrm{v}^2}{2}(\frac{1}{\mathrm{D}^+} - \frac{1}{\mathrm{D}^-})),$$

where $\hat{f}_{(S_t^*,\Gamma_t^{(\alpha^*)})}(y;z,\lambda), \lambda \geq 0,$ *is given by*

$$\hat{f}_{(S_t^*,\Gamma_t^{(\alpha^*)})}(y;z,\lambda) = \int_0^t e^{-\lambda\tau} f_{(S_t^*,\Gamma_t^{(\alpha^*)})}(y;z,\tau)d\tau.$$

Proof. For $c(t,y)$ defined by (2.29), consider the change of concentration given by

$$\tilde{c}(t,y) = e^{-\frac{v}{D(y)}y} c(t,y). \tag{2.35}$$

Then, it is straightforward to show that $\tilde{c}(t,y)$ evolves according to the following skew reaction-dispersion equation

$$\frac{\partial \tilde{c}}{\partial t} = \frac{1}{2}\frac{\partial}{\partial y}(D(y)\frac{\partial \tilde{c}}{\partial y}) - \frac{v^2}{2D(y)}\tilde{c} \tag{2.36}$$

$$\tilde{c}(t,0^+) = \tilde{c}(t,0^-), \qquad D^+\frac{\partial \tilde{c}}{\partial y}(t,0^+) = D^-\frac{\partial \tilde{c}}{\partial y}(t,0^-). \tag{2.37}$$

Moreover, from (2.35),

$$\tilde{c}(0,y) = c_0(y)e^{-\frac{v}{D(y)}y}. \tag{2.38}$$

It now follows from the Feynman-Kac formula that

$$c(t,y) = \mathrm{e}^{\frac{\mathrm{v}}{\mathrm{D(y)}}\mathrm{y}}\tilde{\mathrm{c}}(\mathrm{t},\mathrm{y}) = \mathrm{e}^{\frac{\mathrm{v}}{\mathrm{D(y)}}\mathrm{y}}\mathbb{E}_{\mathrm{y}}\left(\mathrm{c}_0(\mathrm{S}_\mathrm{t}^*)\mathrm{e}^{-\frac{\mathrm{v}}{\mathrm{D}(\mathrm{S}_\mathrm{t}^*)}\mathrm{S}_\mathrm{t}^*}\mathrm{e}^{\left(-\int_0^\mathrm{t}\frac{\mathrm{v}^2}{2\mathrm{D}(\mathrm{S}_\mathrm{r}^*)}\mathrm{dr}\right)}\right), \tag{2.39}$$

where $S_t^*, t \geq 0$, denotes the driftless rescaled (physical) skew Brownian motion defined by (2.33).

In view of the special form (2.31) of the dispersion coefficient, this formula may be reexpressed in terms of the occupation time,

$$\Gamma_t^{(\alpha)} = \int_0^t \mathbf{1}_{[0,\infty)}(B_s^{(\alpha)})ds$$

of skew Brownian motion on the positive axis. Namely,

$$c(t,y) = \mathrm{e}^{\frac{\mathrm{v}}{\mathrm{D(y)}}\mathrm{y}}\mathrm{e}^{-\frac{\mathrm{v}^2}{2\mathrm{D}^-}\mathrm{t}}\mathbb{E}_{\mathrm{y}}\left(\mathrm{c}_0(\mathrm{S}_\mathrm{t}^*)\mathrm{e}^{-\frac{\mathrm{v}}{\mathrm{D}(\mathrm{S}_\mathrm{t}^*)}\mathrm{S}_\mathrm{t}^*}\mathrm{e}^{\left(-\frac{\mathrm{v}^2}{2}(\frac{1}{\mathrm{D}^+}-\frac{1}{\mathrm{D}^-})\Gamma_\mathrm{t}^{(\alpha^*)}\right)}\right). \tag{2.40}$$

From the relation (2.34), it follows that (2.40) may be expressed as

$$c(t,y) = \mathrm{e}^{\left(\frac{\mathrm{v}}{\mathrm{D(y)}}\mathrm{y}-\frac{\mathrm{v}^2}{2\mathrm{D}^-}\mathrm{t}\right)} \times$$
$$\int_0^t \int_{-\infty}^{\infty} c_0(z)\mathrm{e}^{\left(-\frac{\mathrm{v}}{\mathrm{D(z)}}\mathrm{z}\right)}\mathrm{e}^{\left(-\frac{\mathrm{v}^2}{2}\left(\frac{1}{\mathrm{D}^+}-\frac{1}{\mathrm{D}^-}\right)\tau\right)}\mathrm{f}_{(\mathrm{S}^*_\mathrm{t},\Gamma^{(\alpha^*)}_\mathrm{t})}(\mathrm{y};\mathrm{z},\tau)\ \mathrm{dy}\ \mathrm{d}\tau.$$

□

In addition to concentration curves, as noted in the Introduction, breakthrough fluxes have been the subject of recent experiments in which a particularly distinguished asymmetry in breakthrough curves has been reported under mirror symmetric flows from fine to coarse and coarse to fine geometries. The experiments of Berkowitz et al. (2009) were intended to explore the so-called flux-averaged breakthrough concentration curves $c_f(t) = c_f(t,y)$, for fixed y as a function of t, defined by

$$c_f(t,y) = c(t,y) - \frac{D(y)}{2v}\frac{\partial c}{\partial y}, \qquad (2.41)$$

in the presence of the two different configurations (fine-to-coarse and coarse-to-fine) under mirror symmetric reversed flow conditions. Using Theorem 2.5.1, one may explicitly analyze the resulting fluxes defined by (2.41) for observed asymmetries; see, for example, plots in Appuhamillage et al. (2010). While such curves are consistent with experiments, from a probabilistic point of view first passage times provide a more natural formulation of this phenomena. Since the mirror image of velocity is used in the fine to coarse and coarse to fine arrangements, we take $v = 0$ to focus on the pure effect of the interface on dispersion. Also one recall from Remark 2.1.1 that the parameter $\gamma \equiv \gamma(\alpha, v)$ specifying the elastic change of measure is invariant under the transformations $\alpha \to 1-\alpha$, $v \to -v$.

The first symmetry result for concentration profiles provides a point of contrast to first passage times. In addition, it highlights a symmetrization of Walsh's formula (2.11) by the physical diffusion; that is, rescaling space by the respective diffusivities symmetrizes the transition probabilities when $\alpha = \alpha^*$.

Proposition 2.5.2. *Let $p^{(\alpha)}(t,x,y)$ denote the transition probabilities for $\alpha-$skew Brownian motion given in (2.11) and let $p^*(t,x,y)$ denote the transition probabilities for Y in the case $v=0$. Then $p^{(\alpha)}(t,x,y)$ is asymmetric and discontinuous across the interface, while $p^*(t,x,y)$ is symmetric and continuous across the interface.*

Proof. The first assertion follows from inspection of Walsh's formula (2.11) and the second by the indicated change of variables to obtain the transition probabilities of $Y_t = s(B_t^{(\alpha^*)}), t \geq 0$, for $\alpha^* = \frac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}$. Namely, if $y \geq 0$ then

$$p^*(t,x,y) \quad = \quad \begin{cases} \dfrac{2}{\sqrt{D^+}+\sqrt{D^-}}\dfrac{1}{\sqrt{2\pi t}}\mathrm{e}^{\left(-\frac{(\mathrm{y}\sqrt{\mathrm{D}^-}-\mathrm{x}\sqrt{\mathrm{D}^+})^2}{2\mathrm{D}^-\mathrm{D}^+\mathrm{t}}\right)} & \text{if } x \leq 0, \\ \dfrac{1}{\sqrt{2\pi D^+ t}}\left[\mathrm{e}^{\left(-\frac{(\mathrm{y}-\mathrm{x})^2}{2\mathrm{D}^+\mathrm{t}}\right)} + \dfrac{\sqrt{\mathrm{D}^+}-\sqrt{\mathrm{D}^-}}{\sqrt{\mathrm{D}^-}+\sqrt{\mathrm{D}^+}}\mathrm{e}^{\left(-\frac{(\mathrm{y}+\mathrm{x})^2}{2\mathrm{D}^+\mathrm{t}}\right)}\right] & \text{if } x > 0, \end{cases}$$

whereas if $y \leq 0$, then

$$p^*(t,x,y) \quad = \quad \begin{cases} \dfrac{1}{\sqrt{2\pi D^- t}}\left[\mathrm{e}^{\left(-\frac{(\mathrm{y}-\mathrm{x})^2}{2\mathrm{D}^-\mathrm{t}}\right)} - \dfrac{\sqrt{\mathrm{D}^+}-\sqrt{\mathrm{D}^-}}{\sqrt{\mathrm{D}^-}+\sqrt{\mathrm{D}^+}}\mathrm{e}^{\left(-\frac{(\mathrm{y}+\mathrm{x})^2}{2\mathrm{D}^-\mathrm{t}}\right)}\right] & \text{if } x < 0. \\ \dfrac{2}{\sqrt{D^+}+\sqrt{D^-}}\dfrac{1}{\sqrt{2\pi t}}\mathrm{e}^{\left(-\frac{(\mathrm{y}\sqrt{\mathrm{D}^+}-\mathrm{x}\sqrt{\mathrm{D}^-})^2}{2\mathrm{D}^-\mathrm{D}^+\mathrm{t}}\right)} & \text{if } x \geq 0, \end{cases}$$

□

The resulting corollaries to Theorem 2.5.1 establish a simple probabilistic basis for the symmetries and asymmetries predicted by experimental results of Berkowitz et al (2009) and Kuo et al. (1999).

Corollary 2.5.3. *Let $Y^{(\pm v)}$ denote the respective physical skew diffusions with drift v. Then for any $y, t \geq 0$,*

$$P_{-y}(Y_t^{(v)} \in dy) = P_y(Y_t^{(-v)} \in -dy).$$

Proof. In the case $v = 0$, this is the previously noted symmetrization of Walsh's formula given by Proposition 2.5.2, that is, $p^*(t,-y,y) = p^*(t,y,-y)$. The extension to $v \neq 0$ may be checked from Theorem 2.5.1. □

On the other hand, as suggested by Corollary 2.1.6, mirror symmetry of the geometric configuration results in an asymmetric stochastic ordering of the breakthrough times. In particular, *fine to coarse breakthrough is faster than coarse to fine breakthrough*! To isolate the role of the interface in the first passage time between symmetrically configured fine to coarse and coarse to fine media, we take $v = 0$ and consider the fine to coarse configuration.

Lemma 2.5.4. *For $c > 0$, $0 < \alpha < 1$, let $B^{(\alpha)}$ be skew Brownian motion starting at $B_0^{(\alpha)} = 0$. Then the process $\{B_{ct}^{(\alpha)} : t \geq 0\}$ is distributed as $c^{\frac{1}{2}} B^{(\alpha)}$.*

Proof. This follows immediately from the formula (2.11) for the transition probabilities through the finite dimensional distributions of the process started at zero. □

Corollary 2.5.5. *Suppose that $\sqrt{D^-} < \sqrt{D^+}, v = 0$. Let $Y = s(B^{(\alpha^*)})$ denote the corresponding physical diffusion. Also let*

$$T_y^* = \inf\{t \geq 0 : Y_t = y\}.$$

Then for each $t > 0$,

$$P_{-y}(T_y^* > t) < P_y(T_{-y}^* > t).$$

Proof. Without loss of generality take $y = 1$. Using the scaling property from Lemma 2.5.4 and symmetry of Brownian motion, one has

$$T_0^* =^{P_1-\text{dist}} \frac{1}{D^+} T_0, \tag{2.42}$$

and

$$T_0^* =^{P_{-1}-\text{dist}} \frac{1}{D^-} T_0. \tag{2.43}$$

Next, one similarly has

$$T_1^* =^{P_0-\text{dist}} \frac{1}{D^+} T_1^{(\alpha^*)}, \tag{2.44}$$

and

$$T^*_{-1} =^{P_0-\text{dist}} \frac{1}{D^-} T_1^{(1-\alpha^*)}. \tag{2.45}$$

In particular, using the strong Markov property to obtain convolutions, one has

$$P_{-1}(T_1^* > t) = \int_0^t P_0(\frac{1}{D^+} T_1^{(\alpha^*)} > t - s) P_0(\frac{1}{D^-} T_1 \in ds), \tag{2.46}$$

and

$$P_1(T^*_{-1} > t) = \int_0^t P_0(\frac{1}{D^-} T_1^{(1-\alpha^*)} > t - s) P_0(\frac{1}{D^+} T_1 \in ds). \tag{2.47}$$

Now, for $D^- < D^+$, $1 > \alpha^* > 1/2$.. Thus, in view of Corollary 2.1.6, the term $\frac{1}{D^-} T_1 \equiv \frac{1}{D^-} T_1^{(1/2)}$ is stochastically smaller than $\frac{1}{D^-} T_1^{(1-\alpha^*)}$ under P_0, and similarly the term $\frac{1}{D^+} T_1^{(\alpha^*)}$ is stochastically smaller than $\frac{1}{D^+} T_1$ under P_0. The assertion follows by an application of Lemma 2.4.1. □

At the (macro) scale of particle concentrations, the determination of the appropriate parameter $\alpha = \alpha^*$ can be deduced from conservation (continuity) principles; Uffink (1985), Ramirez et al. (2006). However, from a probabilistic point of view we will see that one may also arrive at α^* by two different but related "stochastic balancing principles". One may be viewed in terms of a martingale property, and the other is equivalent to a continuity correction to a local time by the physical skew diffusion. While simple, such principles at the scale of individual particle motions provide a probabilistic basis for possible extensions of the theory to more complex geometries not available at the scale of (2.29). We close by establishing these two "principles".

In establishing these principles, the Itô-Tanaka and the occupation time formulae are repeatedly used. We find it convenient to use the versions of these formulae utilizing the *right local time* of the processes involved. Namely, given a semimartingale Y with quadratic variation denoted by $\langle Y, Y \rangle$ its right local time at a is defined by

$$A_+^Y(t, a) = \lim_{\epsilon \downarrow 0} \frac{1}{\epsilon} \int_0^t \mathbf{1}_{[a \le Y_s < a+\epsilon]} d \langle Y, Y \rangle_s .$$

Recall also that the *left local time*, A_-^Y and the *symmetric local time* L^Y are respectively defined as

$$A_-^Y(t,a) = \lim_{\epsilon \downarrow 0} \frac{1}{\epsilon} \int_0^t \mathbf{1}_{[a-\epsilon<Y_s<a]} d\left\langle Y,Y\right\rangle_s,$$

and

$$L_t^Y(a) = \frac{1}{2}\left[A_+^Y(t,a) + A_-^Y(t,a)\right].$$

In the particular case of skew Brownian motion, the following relations among one sided and the symmetric local times at 0 are known; see, for example, Ouknine (1990).

$$2\alpha L_t^{B^{(\alpha)}}(0) = A_+^{B^{(\alpha)}}(t,0), \quad 2(1-\alpha)L_t^{B^{(\alpha)}}(0) = A_-^{B^{(\alpha)}}(t,0) \tag{2.48}$$

In particular,

$$dB_t^{(\alpha)} = dB_t + \frac{2\alpha-1}{2\alpha} dA_+^{B^{(\alpha)}}(t,0) \tag{2.49}$$

Proof of Theorem 2.1.9 (Martingale Determination of α^*): Recall that $S_t^* = \sqrt{D^+}(B_t^{(\alpha^*)})^+ - \sqrt{D^-}(B_t^{(\alpha^*)})^-$. First, note that with $A_t^*(a) = A_+^{S^*}(t,a)$ one has that at $a = 0$,

$$A_t^*(0) = \sqrt{D^+}\ A_+^{B^{(\alpha^*)}}(t,0). \tag{2.50}$$

Indeed, from the definitions,

$$\begin{aligned} A_t^*(0) &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_0^t \mathbf{1}_{[0\le S_s^*<\epsilon]}\ d\langle S^*,S^*\rangle_s \\ &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_0^t \mathbf{1}_{[0\le B_s^{(\alpha^*)}<\frac{\epsilon}{\sqrt{D^+}}]} D^+\ ds \\ &= \sqrt{D^+}\ A_+^{B^{(\alpha^*)}}(t,0). \end{aligned}$$

We make the claim that in terms of $A_t^*(0)$,

$$dS_t^* = \sqrt{D(B_t^{(\alpha^*)})}\ dB_t + \left(\frac{D^+ - D^-}{2D^+}\right) dA_t^*(0). \tag{2.51}$$

To see this, apply the Itô-Tanaka formula to $(S_t^*)^+$ to get

$$d(S_t^*)^+ = \sqrt{D^+}\Big[\mathbf{1}_{[B_t^{(\alpha^*)}>0]} dB_t + \frac{1}{2} dA_+^{B^{(\alpha^*)}}(t,0)\Big]. \tag{2.52}$$

Similarly, an application of the Itô-Tanaka formula in connection with $(S_t^*)^-$, (2.49), and the fact that the local time of skew Brownian motion is supported at $x = 0$, yields

$$d(S_t^*)^- = \sqrt{D^-}\Big[-\mathbf{1}_{[B_t^{(\alpha^*)}\le 0]}dB_t - \frac{(2\alpha^*-1)}{2\alpha^*}dA_+^{B^{(\alpha^*)}}(t,0) + \frac{1}{2}dA_+^{B^{(\alpha^*)}}(t,0)\Big]. \tag{2.53}$$

Thus, recalling that $\alpha^* = \sqrt{D^+}/[\sqrt{D^-}+\sqrt{D^+}]$, it follows from (2.52), (2.53) that

$$dS_t^* = d(S_t^*)^+ - d(S_t^*)^- = \sqrt{D(B_t^{(\alpha^*)})}\; dB_t + \Big(\frac{D^+ - D^-}{2\sqrt{D^+}}\Big)\; dA_+^{B^{(\alpha^*)}}(t,0). \tag{2.54}$$

The claim now follows as a consequence of (2.54) and (2.50).

Now suppose $f \in \mathcal{D}_{D^\pm}$. Hence, f is the difference of two convex functions and its second generalized derivative is

$$f''(da) = f''(a)da + [f'(0^+) - f'(0^-)]\delta_0 \tag{2.55}$$

From the Itô-Tanaka formula, and using (2.51) (2.55), it follows that

$$\begin{aligned} f(S_t^*) &= f(S_0^*) + \int_0^t f_-'(S_s^*)dS_s^* + \frac{1}{2}\int_{\mathbb{R}} A_t^*(a)f''(da) \\ &= f(x) + \int_0^t f'(S_s^*)\sqrt{D(S_s^*)}\; dB_s + \frac{1}{2}\int_{\mathbb{R}} A_t^*(a)\; f''(a)da \\ &\quad + \frac{D^+ - D^-}{2D^+}\int_0^t f_-'(S_s^*))dA_t^*(0) + \frac{1}{2}\int_{\mathbb{R}} A_t^*(a)\left[f'(0^+) - f'(0^-)\right]\delta_0. \end{aligned} \tag{2.56}$$

By the occupation time formula, and noting that the quadratic variation of S^* is given by $D(S_t^*)dt$,

$$\frac{1}{2}\int_{\mathbb{R}} A_t^*(a)f''(da) = \frac{1}{2}\int_0^t D(S_s^*)f''(S_s^*)ds.$$

The theorem is established once we show that the expression in (2.56) vanishes. To see this, note that this expression is the local time at the origin multiplied by

$$\frac{D^+ - D^-}{2D^+}f'(0^-) + \frac{1}{2}\left[f'(0^+) - f'(0^-)\right] = \frac{1}{2}\left(f'(0^+) - \frac{D^-}{D^+}f'(0^-)\right).$$

This vanishes in light of the interface condition imposed on $f \in \mathcal{D}_{D^\pm}$. $\square$

Proof of Theorem 2.1.10(Continuity Correction to Local Time): Note that as a consequence of (2.48)

$$\frac{A_+^{B^{(\alpha)}}(t,0)}{A_-^{B^{(\alpha)}}(t,0)} = \frac{\alpha}{1-\alpha}.$$

Also, recalling the definition of $s(B^{(\alpha)})$, one obtains

$$\begin{aligned}\tilde{A}_+^{s(B^{(\alpha)})}(t,0) &= \lim_{\epsilon\downarrow 0} \frac{1}{\sqrt{D^+}}\frac{\sqrt{D^+}}{\epsilon}\int_0^t \mathbf{1}_{[0\le B_s^{(\alpha)}<\epsilon/\sqrt{D^+}]}ds \\ &= \frac{1}{\sqrt{D^+}}A_+^{B^{(\alpha)}}.\end{aligned}$$

Similarly,

$$\begin{aligned}\tilde{A}_-^{s(B^{(\alpha)})}(t,0) &= \lim_{\epsilon\downarrow 0} \frac{1}{\sqrt{D^-}}\frac{\sqrt{D^-}}{\epsilon}\int_0^t \mathbf{1}_{[\epsilon/\sqrt{D^-}<B_s^{(\alpha)}<0]}ds \\ &= \frac{1}{\sqrt{D^-}}A_-^{B^{(\alpha)}}.\end{aligned}$$

Thus,

$$\frac{\tilde{A}_+^{s(B^{(\alpha)})}(t,0)}{\tilde{A}_-^{s(B^{(\alpha)})}(t,0)} = \frac{\sqrt{D^-}}{\sqrt{D^+}}\frac{\alpha}{1-\alpha}. \qquad (2.57)$$

The continuity follows if and only if $\alpha = \alpha^* := \frac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}$. □

2.6 Summary and Open Problems

The foundational component of this paper provides an extension of basic probability laws governing the trivariate density of Brownian motion, local time and occupation time and their coordinate projections to those for skew Brownian motion. Along the way the basic Feynman-Kac formula for elastic skew Brownian motion was also obtained. The elastic change of concentration measure to a reaction-dispersion concentration was shown to lead to a closed form determination of the concentration curves and transition probabilities for the physical skew diffusion with drift.

The presence of local time and drift presents new mathematical challenges for both Monte–Carlo numerical simulations and other schemes for numerical computation of the fundamental solution to the advection-dispersion equation or, equivalently, the transition probabilities of the process Y. The Zvonkin transformation, see, for example, Rogers and Williams (1987) for background, was explored in Lejay and Martinez (2006) to remove drift for Monte-Carlo purposes. For the present problem (2.29), this transformation results in a coefficient $\rho(x)$ of the second order operator that their theory requires to be bounded. However, in the present application the coefficient $\rho(x)$ is unbounded, in fact, it grows exponentially. In particular, while some interesting examples are included to illustrate their approach, the particle methods developed in Lejay and Martinez (2006) do not apply to (2.29). Another interesting alternative to the more rigorously developed Itô-Tanaka stochastic calculus, that avoids the use of local time and deals directly with generalized stochastic processes, was somewhat formally explored in LaBolle et al. (2000). A companion analytic approach has also been developed by Portenko (1990) in the context of pde's. The results of the present paper together with those of Portenko (1990) may prove useful in putting some of the ideas in LaBolle et al. (2000) on a more rigorous foundation. It certainly illustrates a rich general problem area.

The main point of the application considered in this paper was to (1) precisely determine the structure of concentration as predicted by Fickian advection-dispersion conservation laws in the presence of a sharp interface orthogonal to the flow direction, and (2) to analyze the role of the interface on breakthrough in terms of first passage times. Part of the goal was to dispel speculation among scientists of a need for refinements to the Fickian conservation laws in this context; see Berkowitz et al. (2008). In particular, it has been rigorously established that the Fickian laws provide general qualitative agreement with symmetries and asymmetries observed in experiments.

A number of interesting directions are possible in connection with applications of this type. Having resolved the principal coordinate directions of flow, it is natural to pursue applications to more complicated geometries; for example, advective-dispersive flow in media with spherical intrusions of contrasting dispersion rates.

The solution provided here also provides a benchmark to test various possible numerical and/or Monte–Carlo particle tracking schemes designed to address interfacial discontinuities. The role of local time presents one of the biggest challenges to Monte–Carlo simulation of particle tracking schemes. The transformation to a skew reaction-dispersion equation together with the Feynman–Kac formula and importance sampling methods may make this theory amenable to Monte–Carlo techniques.

We close by mentioning an important unsolved probability problem related to other types of breakthrough measurements, namely, the explicit determination of first passage time density of a particle injected at -1 to reach 1. An explicit formula for this density is unknown to our best knowledge.

Added in Proof: Since submission and acceptance of this article, a formula for the first passage time distribution of skew Brownian motion was obtained in Appuhamillage and Sheldon (2011).

2.7 First Passage Time of Skew Brownian Motion

This section is organized as follows. In Section 2.7.1, we state the main results. In Section 2.7.2, we develop a coupled construction for two different skew Brownian motion processes with different skew parameters that leads to an important relationship between distributions of ranked excursion heights of the two processes, stated in Theorem 2.7.3. In Section 2.7.3, we prove the main results as corollaries to Theorem 2.7.3.

2.7.1 Preliminaries and Main Results

To set some notation and basic definitions, let $B = \{B_t : t \geq 0\}$ be the *standard Brownian motion* process on a probability space $(\Omega, \mathcal{F}, P)$ and let $J_1, J_2, \ldots$ denote the excursion intervals of the reflected process $\{|B_t| : t \geq 0\}$. For $\alpha \in (0,1)$, let $\{A_m^{(\alpha)} : m =$

$0, 1, \ldots\}$ be a sequence of i.i.d. ± 1 Bernoulli random variables with $P(A_m^{(\alpha)} = 1) = \alpha$. Define the *$\alpha$-skew Brownian motion* process $B^{(\alpha)}$ started at 0 by

$$B_t^{(\alpha)} = \sum_{m=1}^{\infty} \mathbb{I}_{J_m}(t) A_m^{(\alpha)} |B_t|, \tag{2.58}$$

where $\mathbb{I}_S$ denotes the indicator function of the set S.

Now let

$$M_1^{(\alpha)}(t) \geq M_2^{(\alpha)}(t) \geq ... \geq 0$$

be the ranked decreasing sequence of excursion heights $\sup_{s \in J_m \cap [0,t]} B_s^{(\alpha)}$ ranging over all m such that $J_m \cap [0, t]$ is nonempty. Note that a negative excursion has height zero, and that the height of the final excursion is included in the ranked list even if that excursion is incomplete. Our first main result gives the distribution of ranked excursion heights.

Theorem 2.7.1. *Fix $y \geq 0$ and $t > 0$. Then for each $j = 1, 2, ...$, the distribution of $M_j^{(\alpha)}(t)$ is given by the formula*

$$P_0(M_j^{(\alpha)}(t) > y) = \sum_{h=1}^{\infty} 2 \binom{h-1}{j-1} \big(1 - 2\alpha\big)^{h-j} \big(2\alpha\big)^j \big(1 - \Phi((2h-1)y/\sqrt{t})\big),$$

where $\Phi(\cdot)$ is the standard normal distribution function.

Now let

$$T_y^{(\alpha)} = \inf\{s \geq 0 : B_s^{(\alpha)} = y\}$$

denote the first time for α-skew Brownian motion to reach y and let $f^{(\alpha)}(x, y, t)$ denote the first passage time density to y at time t of α-skew Brownian motion started at x. When $\alpha = 1/2$, this is the well known first passage time density $f(x, y, t)$ for Brownian motion (e.g., see page 30 of Bhattacharya and Waymire (2009)):

$$f^{(1/2)}(x, y, t) \equiv f(x, y, t) = \frac{|y - x|}{\sqrt{2\pi}\ t^{3/2}} \exp\Big\{- \frac{(y - x)^2}{2t}\Big\}.$$

Notice that $f^{(\alpha)}(x, y, t)dt = P_x(T_y^{(\alpha)} \in dt)$. Our second main result gives formulae for the first passage time density.

Theorem 2.7.2. *Fix $t > 0$. Then*

$$f^{(\alpha)}(x,y,t) = \begin{cases} g^{(\alpha)}_{x,y}(t) & \text{for } x \le 0 < y \\ g^{(\alpha)}_{-x,y}(t) + \dfrac{1-2\alpha}{2\alpha}\big(g^{(\alpha)}_{x,y}(t) - g^{(\alpha)}_{-x,y}(t)\big) & \\ \qquad + 2\alpha(f(x,y,t) - f(-x,y,t)) & \text{for } 0 < x < y \\ f(x,y,t) & \text{for } 0 < y < x \end{cases}$$

where $g^{(\alpha)}_{x,y}(t) = 2\alpha \sum_{j=1}^{\infty}(1-2\alpha)^{j-1}\dfrac{|x-(2j-1)y|}{\sqrt{2\pi}\ t^{3/2}}\exp\Big\{-\dfrac{(x-(2j-1)y)^2}{2t}\Big\}$ *for* $x < y$.

Remark 2.7.1. *Recently, Harada (Harada (2011)) also computed this first passage time formula using completely different method.*

The cases $0 < y < x$ and $x < y < 0$ in the first passage time density are clear because all paths starting at x reach y without hitting zero and hence they are all Brownian motion paths. In cases, $x \le 0 < y$ and $y < 0 \le x$, all paths must cross zero and densities are obtained as a straightforward corollary of Theorem 2.7.1 and the fact that $P_0(T^{(\alpha)}_y \in dt) = P_0(T^{(1-\alpha)}_{-y} \in dt)$. The situation is most complicated when $0 < x < y$ and $y < x < 0$, and one must consider two types of paths from x to y: those that cross zero, and those that reach y before they reach zero.

Notice that when $\alpha = 1/2$, we recover existing results for standard Brownian motion. Namely, from Theorem 2.7.1, we recover the distribution of ranked excursion heights stated in Theorem 3.1 of Csáki and Hu (2004), and from Theorem 2.7.2 we recover the well known first passage time distribution of standard Brownian motion (this fact is not immediately obvious, but nonetheless true, in most complicated cases when $0 < x < y$ and $y < x < 0$).

2.7.2 Relating excursion heights for $B^{(\alpha)}$ and $B^{(\beta)}$

Let $0 \le \alpha < \beta \le 1$. Consider the following coupled construction of α-skew and β-skew Brownian motion. Let B be the standard Brownian motion process and let $A^{(\beta)} =$

$\{A_m^{(\beta)} : m = 0, 1, \ldots\}$ be independently chosen excursion signs so that Equation (2.58) yields an instance of β-skew Brownian motion.

Next, let $\{A_m^{(\alpha/\beta)}: m = 0, 1, \ldots\}$ be a sequence of i.i.d. ± 1 Bernoulli random variables independent of $A^{(\beta)}$ and B with $P(A_m^{(\alpha/\beta)} = 1) = \alpha/\beta$. Define $A_m^{(\alpha)}$ as follows

$$A_m^{(\alpha)} = \begin{cases} 1 & A_m^{(\beta)} = 1, A_m^{(\alpha/\beta)} = 1, \\ -1 & \text{otherwise.} \end{cases}$$

By construction, the sequence $\{A_m^{(\alpha)} : m = 0, 1, \ldots\}$ consists of i.i.d. ± 1 Bernoulli random variables that are independent of B with $P(A_m^{(\alpha)} = 1) = \alpha$. Hence, by using the variables $A_m^{(\alpha)}$ as the excursion signs in Equation (2.58), we obtain an instance $B^{(\alpha)}$ of α-skew Brownian motion.

We think of this as a two-step process: first, construct $B^{(\beta)}$ by independently setting each excursion of $|B|$ to be positive with probability β; then, for each positive excursion of $B^{(\beta)}$, independently decide whether to keep it positive (with probability α/β), or flip it to be negative (with probability $1 - \alpha/\beta$).

The following theorem is motivated by this coupled construction.

Theorem 2.7.3. *Fix $y \geq 0$, $t > 0$ and $\alpha, \beta \in (0, 1)$. For each $j = 1, 2, ...$, the following relation between ranked excursion heights of α- and β-skew Brownian motions holds.*

$$P_0(M_j^{(\alpha)}(t) > y) = \sum_{h=1}^{\infty} \binom{h-1}{j-1} \left(1 - \tfrac{\alpha}{\beta}\right)^{h-j} \left(\tfrac{\alpha}{\beta}\right)^j P_0(M_h^{(\beta)}(t) > y). \tag{2.59}$$

Before giving the proof of Theorem 2.7.3, we state the following lemma from Pitman and Yor (2001), as we use it in the proof.

Lemma 2.7.1 (Pitman and Yor (2001), Lemma 9)**.** *Let*

$$b_k = \sum_{m=0}^{\infty} \binom{m}{k} a_m, \quad k = 0, 1, ...$$

be the binomial moments of a nonnegative sequence $(a_m,\ m = 0, 1, ...)$. *Let* $B(\theta) := \sum_{k=0}^{\infty} b_k \theta^k$ *and suppose* $B(\theta_1) < \infty$ *for some* $\theta_1 > 1$. *Then*

$$a_m = \sum_{k=0}^{\infty} (-1)^{k-m} \binom{k}{m} b_k, \quad m = 0, 1, ...,$$

where the series is absolutely convergent.

Proof of Theorem 2.7.3. For $\alpha < \beta$, we have by the two-step construction of the excursion sign $A_m^{(\alpha)}$ that $M_j^{(\alpha)}(t) = M_{H_j}^{(\beta)}(t)$, where H_j has a negative binomial distribution:

$$P(H_j = h) = \binom{h-1}{j-1} \left(1 - \tfrac{\alpha}{\beta}\right)^{h-j} \left(\tfrac{\alpha}{\beta}\right)^j.$$

Hence

$$P_0(M_j^{(\alpha)}(t) > y) = \sum_{h=1}^{\infty} \binom{h-1}{j-1} \left(1 - \tfrac{\alpha}{\beta}\right)^{h-j} \left(\tfrac{\alpha}{\beta}\right)^j P_0(M_h^{(\beta)}(t) > y). \tag{2.60}$$

For $\beta < \alpha$, the relation can be inverted by an application of Lemma 2.7.1. Let $k := j - 1$ and $m := h - 1$. Then one can write (2.59) as

$$P_0(M_{k+1}^{(\alpha)}(t) > y) = \sum_{m=0}^{\infty} \binom{m}{k} \left(1 - \tfrac{\alpha}{\beta}\right)^{m-k} \left(\tfrac{\alpha}{\beta}\right)^{k+1} P_0(M_{m+1}^{(\beta)}(t) > y). \tag{2.61}$$

We then apply Lemma 2.7.1 to the sequences

$$b_k := \left(1 - \tfrac{\alpha}{\beta}\right)^k \left(\tfrac{\alpha}{\beta}\right)^{-k-1} P_0(M_{k+1}^{(\alpha)}(t) > y), \quad a_m := \left(1 - \tfrac{\alpha}{\beta}\right)^m P_0(M_{m+1}^{(\beta)}(t) > y).$$

After simplifying, we obtain

$$P_0(M_j^{(\beta)}(t) > y) = \sum_{h=1}^{\infty} \binom{h-1}{j-1} \left(1 - \tfrac{\beta}{\alpha}\right)^{h-j} \left(\tfrac{\beta}{\alpha}\right)^j P_0(M_h^{(\alpha)}(t) > y). \tag{2.62}$$

□

2.7.3 Proofs of Main Theorems

We now observe that the main results announced in the introduction will follow as corollaries to Theorem 2.7.3. We first prove the Theorem 2.7.1.

Proof of Theorem 2.7.1. By Theorem 3.1 in Csáki and Hu (2004),

$$P_0(M_j^{(1/2)}(t) > y) = 2\Big(1 - \Phi\Big((2j-1)\frac{y}{\sqrt{t}}\Big)\Big) \tag{2.63}$$

The result is immediate from Theorem 2.7.3 by taking $\beta = 1/2$ in (2.59). □

We now use Theorem 2.7.1 and the following corollary to compute the distribution of first passage time asserted in Theorem 2.7.2.

Corollary 2.7.2. *Fix $t > 0$. Then*

$$P_0(T_y^{(\alpha)} \in dt) = \begin{cases} 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} \frac{(2h-1)y}{\sqrt{2\pi}\ t^{3/2}} \exp\Big\{-\ \frac{((2h-1)y)^2}{2t}\Big\}\ dt & \text{for } y > 0 \\ 2(1-\alpha) \sum_{h=1}^{\infty} (2\alpha-1)^{h-1} \frac{(2h-1)(-y)}{\sqrt{2\pi}\ t^{3/2}} \exp\Big\{-\ \frac{((2h-1)y)^2}{2t}\Big\}\ dt & \text{for } y < 0 \end{cases} \tag{2.64}$$

Proof. For the case $y > 0$ and $t > 0$, we have the following relation between the distributions of $T_y^{(\alpha)}$ and the highest excursion of skew Brownian motion started at 0:

$$P_0(T_y^{(\alpha)} < t) = P_0(M_1^{(\alpha)}(t) > y).$$

Thus using Theorem 2.7.1, one has

$$\begin{aligned} P_0(T_y^{(\alpha)} < t) &= P_0(M_1^{(\alpha)}(t) > y) \\ &= 4\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} \int_{\frac{(2h-1)y}{\sqrt{t}}}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\Big\{-\frac{z^2}{2}\Big\}\ dz. \end{aligned}$$

The result is immediate after taking the derivative of the above expression with respect to t.

For the case $y < 0$, use the relation $P_0(T_y^{(\alpha)} \in dt) = P_0(T_{-y}^{(1-\alpha)} \in dt)$ and the case $y > 0$.

□

Proof of Theorem 2.7.2. Let $T_y \equiv T_y^{(1/2)}$ denote the first time for standard Brownian motion to reach y. Recalling that $P_0(T_y \in dt) = \frac{|y|}{\sqrt{2\pi}\ t^{3/2}} \exp\Big\{-\ \frac{y^2}{2t}\Big\}\ dt$; e.g. see page 30 in Bhattacharya and Waymire (2009), one can write equation (2.64) as

$$P_0(T_y^{(\alpha)} \in dt) = \begin{cases} 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} P_0(T_{(2h-1)y} \in dt) & \text{for } y > 0 \\ 2(1-\alpha) \sum_{h=1}^{\infty} (2\alpha-1)^{h-1} P_0(T_{(2h-1)y} \in dt) & \text{for } y < 0 \end{cases} \tag{2.65}$$

Now note that $T_0^{(\alpha)}$ is distributed as T_0 under P_x for $x \neq 0$, $0 < \alpha < 1$. So clearly for $t > 0$, one has

$$P_x(T_0^{(\alpha)} > t) = P_x(T_0 > t).$$

We prove the case $y > 0$ in the Theorem 2.7.2. The case $y < 0$ is similar.

Case $x \leq 0 < y$:

Using the strong Markov property of skew Brownian motion,

$$P_x(T_y^{(\alpha)} > t) = \int_0^t P_x(T_0 > t-s) P_0(T_y^{(\alpha)} \in ds). \tag{2.66}$$

Then from the first case of equation (2.65), one has

$$\begin{aligned} P_x(T_y^{(\alpha)} > t) &= 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} \int_0^t P_x(T_0 > t-s) P_0(T_{(2h-1)y} \in ds) \\ &= 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} P_x(T_{(2h-1)y} > t) \end{aligned} \tag{2.67}$$

By differentiating the above expression with respect to t and recalling $P_x(T_y \in dt) = \frac{|y-x|}{\sqrt{2\pi}\ t^{3/2}} \exp\Big\{-\ \frac{(y-x)^2}{2t}\Big\}\ dt$, one has

$$P_x(T_y^{(\alpha)} \in dt) = 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} \frac{|x-(2h-1)y|}{\sqrt{2\pi}\ t^{3/2}} \exp\Big\{-\ \frac{(x-(2h-1)y)^2}{2t}\Big\}\ dt \tag{2.68}$$

Case $0 < x < y$:

Observe that

$$P_x(T_y^{(\alpha)} \in dt) = P_x(T_y^{(\alpha)} \in dt, (T_0^{(\alpha)} \leq t)) + P_x(T_y^{(\alpha)} \in dt, (T_0^{(\alpha)} > t)) \tag{2.69}$$

We state the following formula for $P_x(T_0 \in dt, (T_y > t))$ without proof. One can use the heat equation with diffusion equals constant 1 and absorbing boundary conditions at 0 and y to compute the formula. In Feller (1968) (page 296), it has a formula for this probability interms of *sin* series.

$$P_x(T_0 \in dt, (T_y > t)) = P_0(T_x \in dt) + \sum_{m=1}^{\infty} \Big(P_0(T_{2my+x} \in dt) - P_0(T_{2my-x} \in dt) \Big) \quad (2.70)$$

Since the skew Brownian motion is Brownian motion until it reaches zero for the first time and from the reflection principle of Brownian motion, one can write the second term of the right hand side of equation (2.69) using equation (2.70) as follows:

$$\begin{aligned} P_x(T_y^{(\alpha)} \in dt, (T_0^{(\alpha)} > t)) &= P_x(T_y \in dt, (T_0 > t)) \\ &= P_{y-x}(T_0 \in dt, (T_y > t)) \\ &= P_0(T_{y-x} \in dt) \\ &\quad + \sum_{m=1}^{\infty} \Big(P_0(T_{(2m+1)y-x} \in dt) - P_0(T_{(2m-1)y+x} \in dt) \Big) \end{aligned} \quad (2.71)$$

For the first term of the right hand side of equation (2.69), notice that

$$\begin{aligned} &P_x(T_0^{(\alpha)} < T_y^{(\alpha)} < t) \\ &\quad = \mathbb{E}_x \Big[\mathbf{1}_{[T_0^{(\alpha)} < T_y^{(\alpha)} < t]} \Big] \\ &\quad = \mathbb{E}_x \Big[\mathbb{E}_x \Big[\mathbf{1}_{[T_0^{(\alpha)} < T_y^{(\alpha)} < t]} | T_0^{(\alpha)}, \mathbf{1}_{[T_0^{(\alpha)} < T_y^{(\alpha)}]} \Big] \Big] \\ &\quad = \int_0^t \mathbb{E}_x \Big[\mathbf{1}_{[T_0^{(\alpha)} < T_y^{(\alpha)} < t]} | T_0^{(\alpha)} = s, \mathbf{1}_{[T_0^{(\alpha)} < T_y^{(\alpha)}]} \Big] P_x(T_0^{(\alpha)} \in ds, (T_0^{(\alpha)} < T_y^{(\alpha)})) \\ &\quad + \int_0^t \mathbb{E}_x \Big[\mathbf{1}_{[T_0^{(\alpha)} < T_y^{(\alpha)} < t]} | T_0^{(\alpha)} = s, \mathbf{1}_{[T_0^{(\alpha)} \geq T_y^{(\alpha)}]} \Big] P_x(T_0^{(\alpha)} \in ds, (T_0^{(\alpha)} \geq T_y^{(\alpha)})) \end{aligned}$$

Using the strong Markov property of skew Brownian motion and since

$$\mathbb{E}_x \Big[\mathbf{1}_{[T_0^{(\alpha)} < T_y^{(\alpha)} < t]} | T_0^{(\alpha)} = s, \mathbf{1}_{[T_0^{(\alpha)} \geq T_y^{(\alpha)}]} \Big] = 0,$$

one has

$$\begin{aligned} P_x(T_0^{(\alpha)} < T_y^{(\alpha)} < t) &= \int_0^t \mathbb{E}_0 \Big[\mathbf{1}_{[T_y^{(\alpha)} < t-s]} \Big] P_x(T_0^{(\alpha)} \in ds, (T_0^{(\alpha)} < T_y^{(\alpha)})) \\ &= \int_0^t P_0(T_y^{(\alpha)} < t-s) P_x(T_0^{(\alpha)} \in ds, (T_0^{(\alpha)} < T_y^{(\alpha)})) \end{aligned}$$

Using equation (2.65) and again from the fact that the skew Brownian motion is Brownian motion until it reaches zero for the first time, and $P_x(T_0^\alpha < T_y^\alpha) = P_x(T_0 < T_y)$ (note here $0 < x < y$), one has

$$
\begin{aligned}
&P_x(T_0^{(\alpha)} < T_y^{(\alpha)} < t) \\
&\quad = \int_0^t 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} P_0(T_{(2h-1)y} < t-s) P_x(T_0 \in ds, (T_0 < T_y)) \\
&\quad = 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} \int_0^t P_0(T_{(2h-1)y} < t-s) P_x(T_0 \in ds, (T_0 < T_y)) \\
&\quad = 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} \int_0^t P_0(T_{(2h-1)y} < t-s) \\
&\qquad \times \left[P_0(T_x \in ds) + \sum_{m=1}^{\infty} \Big(P_0(T_{2my+x} \in ds) - P_0(T_{2my-x} \in ds) \Big) \right] \\
&\quad = 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} P_0(T_{(2h-1)y+x} < t) \\
&\qquad + \; 2\alpha \sum_{m=1}^{\infty} \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} \Big(P_0(T_{(2(m+h)-1)y+x} < t) - P_0(T_{(2(m+h)-1)y-x} < t) \Big) \\
&\quad = 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} P_0(T_{(2h-1)y+x} < t) \\
&\qquad + \; \sum_{l=2}^{\infty} \big(1 - (1-2\alpha)^l\big) \Big(P_0(T_{(2l-1)y+x} < t) - P_0(T_{(2l-1)y-x} < t) \Big)
\end{aligned}
$$

The second equality is from the strong Markov property of Brownian motion and the last equality is by renaming the index of the double sum.

Thus we have

$$
\begin{aligned}
P_x(T_y^{(\alpha)} \in dt, (T_0^{(\alpha)} \le t)) &= 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} P_0(T_{(2h-1)y+x} \in dt) \\
&\quad + \sum_{l=2}^{\infty} \big(1 - (1-2\alpha)^l\big) \Big(P_0(T_{(2l-1)y+x} \in dt) - P_0(T_{(2l-1)y-x} \in dt) \Big) \qquad (2.72)
\end{aligned}
$$

Then from equations (2.69), (2.71) and (2.72) one has

$$
\begin{aligned}
&P_x(T_y^{(\alpha)} \in dt) \\
&\quad = 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} P_0(T_{(2h-1)y+x} \in dt) \\
&\qquad + \sum_{l=2}^{\infty} \big(1-(1-2\alpha)^l\big)\Big(P_0(T_{(2l-1)y+x} \in dt) - P_0(T_{(2l-1)y-x} \in dt)\Big) \\
&\qquad + P_0(T_{y-x} \in dt) + \sum_{m=1}^{\infty} \Big(P_0(T_{(2m+1)y-x} \in dt) - P_0(T_{(2m-1)y+x} \in dt)\Big) \\
&\quad = 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} P_0(T_{(2h-1)y+x} \in dt) \\
&\qquad + \sum_{l=2}^{\infty} \big(1-(1-2\alpha)^l\big)\Big(P_0(T_{(2l-1)y+x} \in dt) - P_0(T_{(2l-1)y-x} \in dt)\Big) \\
&\qquad + P_0(T_{y-x} \in dt) + \sum_{r=2}^{\infty} P_0(T_{(2r-1)y-x} \in dt) - \sum_{m=1}^{\infty} P_0(T_{(2m-1)y+x} \in dt) \\
&\quad = 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} P_0(T_{(2h-1)y+x} \in dt) \\
&\qquad - \sum_{l=2}^{\infty} (1-2\alpha)^l \Big(P_0(T_{(2l-1)y+x} \in dt) - P_0(T_{(2l-1)y-x} \in dt)\Big) \\
&\qquad + P_0(T_{y-x} \in dt) - P_0(T_{y+x} \in dt) \\
&\quad = 2\alpha \sum_{h=1}^{\infty} (1-2\alpha)^{h-1} P_0(T_{(2h-1)y+x} \in dt) \\
&\qquad - \sum_{l=1}^{\infty} (1-2\alpha)^l \Big(P_0(T_{(2l-1)y+x} \in dt) - P_0(T_{(2l-1)y-x} \in dt)\Big) \\
&\qquad + 2\alpha P_0(T_{y+x} \in dt) - 2\alpha P_0(T_{y-x} \in dt)
\end{aligned}
$$

Case $0 < y < x$:

Notice that, in this case all skew Brownian motion paths till the first passage time to y are away from 0. Thus we have

$$
P_x(T_y^{(\alpha)} \in dt) = \frac{|y-x|}{\sqrt{2\pi} t^{3/2}} \exp\Big\{-\frac{(y-x)^2}{2t}\Big\}\, dt.
$$

□

3 SOLUTE TRANSPORT ACROSS AN INTERFACE: A FICKIAN THEORY FOR SKEWNESS IN BREAKTHROUGH CURVES

This chapter consists of a manuscript of a published paper and author's own work under the supervision of Professor Enrique Thomann.

- **Section 3.1 through 3.5 :** consists of the manuscript
  - Solute Transport Across an Interface: A Fickian Theory of Skewness in Breakthrough Curves by T.A. Appuhamillage, V.A. Bokil, E. Thomann, E. Waymire, B.D. Wood that appeared in *Water Resources Research*, Vol. 46, No. 7, W07511, 2010. doi:10.1029/2009WR008258.

- **Section 3.6 :** This section is an addition to the manuscript presented in Sections 3.1-3.5. Here we present the analysis of occupation times in the presence of a sharp interface.

3.1 Introduction

The convective-dispersive movement of solutes through porous media in the presence of a discontinuous interface (e.g., separating fine and coarse regions) is a topic of both active experimental and theoretical interest (Hoteit et al., 2002; Berkowitz et al., 2009; LaBolle et al., 1998, 2000; Ramirez et al., 2006, 2008). Precise breakthrough measurements in such systems can be experimentally difficult to achieve, and numerical computations in the presence of discontinuous dispersion coefficients can be quite challenging.

Recently, a mathematically rigorous approach was developed by Ramirez et al. (2006, 2008) to represent the solution to solute transport near a discontinuous interface governed by (deterministic) Fickian laws of convection-dispersion in terms of the probability distribution of a special stochastic particle motion. This was then used to analyze solute transport for the case of flow parallel to the discontinuous interface. In that work it was shown that, while the solute particle coordinates in the direction of the flow are convected Brownian motions, the coordinate across the interface is a rescaled α-skew Brownian motion for a particular (physical) value of the parameter α. It is important to emphasize here that the transport model itself is deterministic; the geometry, physical properties, constitutive relations, and boundary conditions associated with the domain are assumed *a priori* to be known with certainty. Stochastic particle motions enter as a mathematical tool for analyzing the solution to the partial differential equations (PDEs) that define the solute transport process within this domain. A useful analogy can be made here with the process of pure molecular diffusion in a homogeneous domain. The diffusion process can be represented by either a parabolic (heat-type) equation defined with constant coefficients defined throughout the domain, or it can be represented as an ensemble of stochastic particle motions whose (Gaussian) distribution satisfies the corresponding PDE. This equivalence has been recognized for over a century, and hydrologists have used these ideas effectively for decades (a lucid discussion of this equivalence is given in Kac (1947), for example). It is also important to note that, for the work reported here, the Fickian constitutive relation for describing dispersive fluxes is applied only in homogeneous sub-regions of the domain, where it is well established that such a constitutive relations are correct. This does not imply, however, that the observation of transport for the domain taken as a whole should be expected to obey a Fickian flux law via the definition of an effective dispersion coefficient. Our results, in fact, show that this is not the case for transport perpendicular to a sharp interface. It is interesting that a notion of skew Brownian motion introduced in the mathematics literature by Itô and McKean (1963), while the discrete counterpart of skew random walk found its way into the hydrology literature through the classic work of Uffink (1985). Much of the intuition underlying the more technically difficult concepts involved in the continuous space-time skew Browian motion are conceptually accessible in terms of the skew random walk discretization.

The derivation of α-skew Brownian motion as the underlying stochastic particle motion governing the (deterministic) Fickian convection-dispersion concentration field in the presence of the sharp interface *parallel* to the mean direction of flow allowed us to obtain a closed-form solution for the evolution of the concentration field in space and time. In addition this development provided a well-founded approach for implementing Monte-Carlo stochastic particle methods in the presence of such discontinuities, and it confirmed experimental results of Hoteit et al. (2002). A key technical point with regard to this previous result is the absence of drift in the particle coordinate associated with the α-skew Brownian motion.

Flow orthogonal to an interface presents new challenges for the use of α-skew Brownian motions. The purpose of the present paper is to extend our previous theory to this case. Our approach involves a combination of mathematical methods from probability and partial differential equations; however the basic physical model for concentration being analyzed is still the standard (deterministic) Fickian model of convection-dispersion. As in the case for flow parallel to the interface, we have now obtained an explicit solution for the concentration field for the case of flow perpendicular to the interface. While the solution is expressed in terms of classic exponential and Gauss error functions (available in standard computational libraries such as MATLAB$^{\text{TM}}$or Mathematica$^{\text{TM}}$), the expression is substantially more complicated algebraically than the analogous expression for the case of flow parallel to the interface. Ultimately, a general theory that provides particle representations for solute transport in discontinuous media would need to provide a model involving interfaces whose surface might be in any orientation relative to the local fluid velocity vector.

As an application, we use this new theory to explain certain symmetries and asymmetries that have been recently observed in the flux-averaged breakthrough curves measured for a 1-dimensional porous medium system with a discontinuity in the dispersion coefficient perpendicular to the direction of the mean velocity. Experiments of Berkowitz et al. (2009) involving breakthrough times of a conservative tracer across an interface between two porous media have uncovered interesting symmetry and asymmetry properties in the resident versus flux-averaged concentration curves. Specifically, the experimental breakthrough curves for the flux-averaged concentration exhibit a significant asymmetry under a mirror-symmetric distribution of two media. In other words, the flux-averaged breakthrough curves for transport in the direction of coarse-to-fine media is different from the breakthrough curve obtained in the direction of fine-to-coarse media (the breakthrough curves for the *resident* concentration, by comparison, are symmetric). Such observations about the reciprocity for the breakthrough curve when the the direction of flow is reversed have been reported previously (e.g., Kuo et al. (1999b); Sternberg et al. (1996); Berentsen et al. (2005); Cortis and Zoia (2009)). In particular, Kuo et al. (1999b) explicitly noted that for one-dimensional experiments conducted in their laboratory, the solute breakthrough curve that was obtained in the presence of discontinuous (coarse-fine) media was different when the direction of flow was changed.

In this paper we demonstrate mathematically that such symmetries and asymmetries, respectively, are precisely predicted by Fickian laws of dispersion. This is possible due to the explicit form of the solution obtained here. Graphs are provided for graphical illustration of these results.

In Section 3.2 the mathematical formulation of the (Fickian) convection-dispersion equation in the presence of discontinuous dispersion coefficients is introduced, and a corresponding stochastic particle motion is obtained via a combination of a transformation on the drift, made simpler for the case of steady velocity assumed here, and the Feynman-Kac formula. In particular, the concentration curve is explicitly represented as an expected value of a functional of an exponentially killed skewed Brownian particle as a result. The problem of computing this expectation is then taken up in the Section 3.3. It is solved by an application of some recent mathematical developments in a companion paper by Appuhamillage et al. (2011b) on the trivariate density of skew Brownian motion, its local time, and its occupation time. While many of the technical details are beyond the intended scope of this article, an effort is made to make the concepts and resulting computations physically plausible. In Section 3.4, the application of the resulting formulae are used to examine symmetries in the transient concentration and asymmetries in flux-averaged breakthrough curves. Finally, a discussion of the relevance of these formulae to related research in numerical methods, as well as future directions involving more complex interface geometries is given in Section 3.5.

3.2 Fickian Model of Advection-Dispersion Across a Sharp Interface

Consider an initial concentration of inert tracer $c_0(\mathbf{y}), \mathbf{y} \in R^d$, under a uniform (and thus incompressible) velocity field $\mathbf{v}$ and with dimensions $d = 1, 2$ or 3 . We have selected a right-hand coordinate system in which y_2 is the vertical coordinate axis, and $y_1 - y_3$ the plane coordinate axes (Fig 3.1).

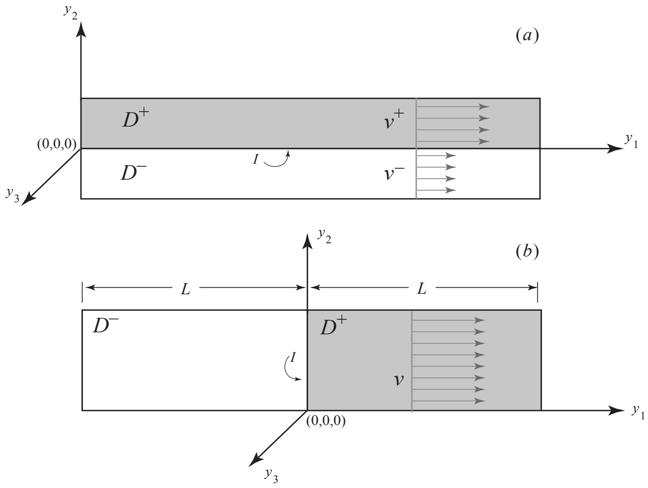

FIGURE 3.1: Coordinate system convention used for this work. (a) The system geometry analyzed previously by *Ramirez et al., 2008.* (b) The system geometry examined in the present work.

In $d = 3$ take $\mathbf{v} = (v, 0, 0)$, while for $d = 2, \mathbf{v} = (v, 0)$, and for $d = 1, \mathbf{v} = v$ is a positive (constant) scalar. With these choices, the flow is parallel to an interface defined by a discontinuity in the dispersion across $y_2 = 0$ [Fig 3.1a], and the flow is orthogonal to an interface defined by a discontinuity across $y_1 = 0$ [Fig 3.1b].

Under a Fickian flux law the corresponding concentration, $c(\mathbf{y}, t)$, evolves according to the linear, possibly non-homogeneous, parabolic equation in divergence form

$$\frac{\partial c}{\partial t} = \nabla \cdot (\mathbf{D}(\mathbf{y}) \cdot \nabla c(\mathbf{y}, t)) - \nabla \cdot (\mathbf{v} c(\mathbf{y}, t)) \tag{3.1}$$

$$c(\mathbf{y}, 0) = c_0(\mathbf{y}), \quad \mathbf{y} \in R^d \tag{3.2}$$

where $\mathbf{D}(\mathbf{y})$ is the effective dispersion tensor. Note that in equations (3.1) and (3.2) pore-scale physics has already been homogenized (i.e. it is an inherently continuum representation), and the demand is assumed to be unbounded. In discontinuous media, two other conditions are required at the interface between the media types. Across the interface, I, the conservation of mass requires the continuity of flux; similarly, within the Fickian framework the concentration is also required to be continuous across the interface. Together, these conditions imply

$$\mathbf{n} \cdot \mathbf{D}^{+}(\mathbf{y}) \cdot \nabla c(\mathbf{y}, t)|_{\mathbf{y} \in I^{+}} = \mathbf{n} \cdot \mathbf{D}^{-}(\mathbf{y}) \cdot \nabla c(\mathbf{y}, t)|_{\mathbf{y} \in I^{-}} \tag{3.3}$$

$$c(\mathbf{y}, t)|_{\mathbf{y} \in I^{+}} = c(\mathbf{y}, t)|_{\mathbf{y} \in I^{-}}. \tag{3.4}$$

Here $\mathbf{n}$ denotes a normal vector (pointing in the positive y_1-direction) to the interface, I, and I^{+} and I^{-} indicate the appropriate directions for evaluation of the one-sided derivatives at the discontinuity. In the case to be considered here, when the y_1 coordinate axis is aligned with the mean velocity vector, one may write the dispersion tensor $\mathbf{D}(\mathbf{y})$ in terms of a scalar longitudinal (D) dispersion coefficient and transverse (D_T) dispersion coefficient, respectively, via the diagonal matrix

$$\mathbf{D}(\mathbf{y}) = \begin{bmatrix} D(\mathbf{y}) & 0 & 0 \\ 0 & D_T(\mathbf{y}) & 0 \\ 0 & 0 & D_T(\mathbf{y}) \end{bmatrix} \tag{3.5}$$

We emphasize here that the symbol $D(\mathbf{y})$ is the total longitudinal effective dispersion coefficient, and it includes the effects of both diffusion and mechanical dispersion.

The case of three-dimensional flow in the direction of $\mathbf{e}_1 = (1, 0, 0)$ and parallel to a plane interface $I(\mathbf{y})$ (*e.g.*, $I(\mathbf{y}) \equiv \{\mathbf{y} : y_2 = 0\}$), in the aforementioned paper by Ramirez et al. (2006) is defined in the context of (3.1) by (Fig 3.1a)

$$D(\mathbf{y}) = \begin{cases} D^{+} & \text{if} \quad y_2 \geq 0 \\ D^{-} & \text{if} \quad y_2 < 0. \end{cases} \tag{3.6}$$

However, the focus of the present paper is that of an orthogonal plane interface $I(\mathbf{y}) \equiv \{\mathbf{y} : y_1 = 0\}$ for the same flow defined by (Fig 3.1b)

$$D(\mathbf{y}) = \begin{cases} D^{-} & \text{if} \quad y_1 < 0. \\ D^{+} & \text{if} \quad y_1 \geq 0 \end{cases} \tag{3.7}$$

3.2.1 Stochastic Particle Motions for Transport Across a Discontinuous Interface

3.2.1.1 Brownian Motion

Just as Einstein's theory of Brownian motion is intrinsically associated with the diffusion equation through its probability distribution in space and time, a basic connection exists between more general convection-dispersion equations and stochastic particle motions. In particular the appropriate transition probabilities for the particles representing the concentration field can be derived for cases where there are discontinuities in the macroscale properties of the porous medium.

In the stochastics literature, the balance equation given by Eq (3.1) is usually written in the following form

$$\frac{\partial c}{\partial t} = \sum_{i=1}^{d} \sum_{j=1}^{d} \frac{\partial^2}{\partial y_i \partial y_j} (D_{ij}(\mathbf{y}) c) - \sum_{i=1}^{d} \frac{\partial}{\partial y_i} (u_i(\mathbf{y}) c), \tag{3.8}$$

It is easy to verify that this is a simple rearrangement of Eq (3.1), and that it is otherwise equivalent. In this expression, the new drift $\mathbf{u}$ involves both the macroscopic flow field $\mathbf{v} = (v_1, \ldots, v_d)$, and the microscopic dispersive drift due to heterogeneity in the dispersion coefficient field $\mathbf{D}(\mathbf{y}) = [D_{ij}(\mathbf{y})]_{1 \leq i,j \leq d}$. This is given by the general relationships

$$u_i(\mathbf{y}) = v_i + \sum_{j=1}^{d} \frac{\partial}{\partial y_j} D_{ij}(\mathbf{y}) \quad i = 1, 2, \ldots, d. \tag{3.9}$$

The particle motions can themselves be described in terms of stochastic differential equations involving the same dispersion tensor and drift. For smooth coefficients the continuous motion of particles holds the coefficients approximately constant in infinitesimal time. As a result, the Itô calculus provides a description under which the particles evolve locally (small time) as rescaled Brownian particles with drift, but as time evolves the rescaling and drift continuously change. That is

$$d\mathbf{Y} = \mathbf{u}(\mathbf{Y}(t))dt + [2\mathbf{D}(\mathbf{Y}(t))]^{\frac{1}{2}} \cdot d\mathbf{B}(t). \tag{3.10}$$

Note that Eq (3.10) applies at the same scale as the differential balance given by Eq (3.1); in fact, one must interpret Eq (3.10) as the stochastic particle analogue to the differential equation given in Eq (3.1). In other words, the particle motions in this case have the statistics that reproduce the macroscale effective dispersion tensor, $\mathbf{D}(\mathbf{y})$.

For non-smooth coefficients, a different physical and mathematical model must be adopted in order to correctly capture particle dynamics at the interface. The theory of Brownian motion applies to homogeneous media with constant coefficients, however the discontinuity in dispersivity at the interface affects the basic motion. The resulting particle motions, called α-skew Brownian motions, are no-longer Gaussian distributed as is evident in Eq. (3.12) below. As a result of the skewness, control of the interface flux (3.3) has a stochastic counterpart in terms of so-called *local time* that appears in the stochastic differential equation. Thus, for the stochastic particle motions the local time is intrinsic to the description of their movement. The intrinsic presence of local time has significant implications for numerical Monte-Carlo particle simulations discussed at the conclusion of this paper.

3.2.1.2 $\alpha-$Skew Brownian Motion

The α-skew Brownian motion was introduced in the mathematics literature in Itô and McKean (1963) according to the following prescription. Consider a one-dimensional standard Brownian motion $B(t), t \geq 0$, starting at $B(0) = 0$. The Brownian motion process reflected at 0 is then represented by the absolute value $|B(t)|, t \geq 0$. To construct the $\alpha-$skew Brownian motion, denoted $B^{(\alpha)}(t), t \geq 0$, for a parameter $0 \leq \alpha \leq 1$, one first enumerates the intervals between pairs of consecutive zeroes of $|B(t)|, t \geq 0$, as the random intervals $J_1, J_2, \ldots$ (Fig 3.2). While these intervals can be enumerated, they can not be ordered; in Fig 3.2, no particular order is intended.

Next let $A_1, A_2, \ldots$ be an independent, identically distributed sequence of Bernoulli ± 1 trials, independent of the Brownian motion, with $P(A_n = +1) = \alpha$, $P(A_n = -1) = 1 - \alpha, n \geq 1$. Now define

$$B^{(\alpha)}(t) = A_n |B(t)|, \qquad t \in J_n, \quad n = 1, 2, \ldots. \tag{3.11}$$

That is, the sign of an excursion of $|B(t)|, t \in J_n$ is changed from $+$ to $-$ with probability $1 - \alpha$, independently from excursion to excursion (Fig 3.2). The parameter α is referred to as a "transmission probability". In the case $\alpha = \frac{1}{2}$, one recovers a Brownian motion as $B^{(\frac{1}{2})}(t), t \geq 0$. The two other special cases are $\alpha = 1$, in which $B^{(1)}(t), t \geq 0$, is the Brownian motion reflected to the right of 0, and $\alpha = 0$, in which case $B^{(0)}(t), t \geq 0$, is the Brownian motion process reflected to the left of 0.

The resulting $\alpha-$skew Brownian motion is a Markov process with continuous sample paths whose transition probabilities $p^{(\alpha)}(y_0, y; t)$ were computed by Walsh (1978) via judicious applications of the reflection principle for Brownian motion. We record the result here for ease of reference

$$p^{(\alpha)}(y_0, y; t) \quad = \quad \begin{cases} \frac{1}{\sqrt{2\pi t}} e^{-\frac{(y-y_0)^2}{2t}} + \frac{(2\alpha-1)}{\sqrt{2\pi t}} e^{-\frac{(y+y_0)^2}{2t}} & \text{if } y_0 > 0, y > 0 \\ \frac{1}{\sqrt{2\pi t}} e^{-\frac{(y-y_0)^2}{2t}} - \frac{(2\alpha-1)}{\sqrt{2\pi t}} e^{-\frac{(y+y_0)^2}{2t}} & \text{if } y_0 < 0, y < 0 \\ \frac{2\alpha}{\sqrt{2\pi t}} e^{-\frac{(y-y_0)^2}{2t}} \quad \text{if } y_0 \leq 0, y > 0 \\ \frac{2(1-\alpha)}{\sqrt{2\pi t}} e^{-\frac{(y-y_0)^2}{2t}} \quad \text{if } y_0 \geq 0, y < 0. \end{cases} \tag{3.12}$$

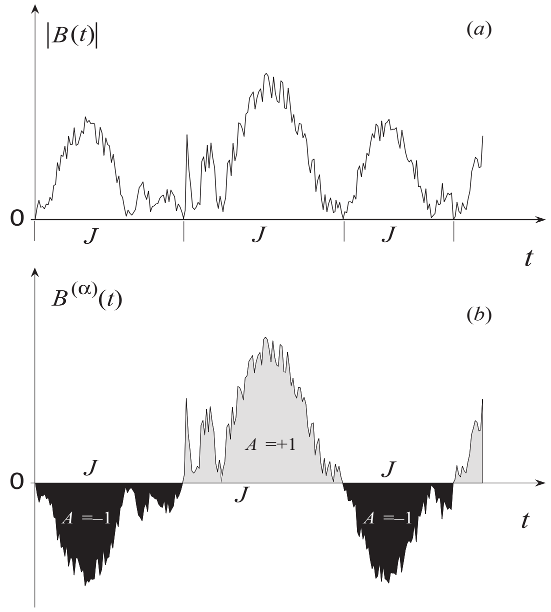

FIGURE 3.2: (a) A standard Brownian motion (reflected at the origin) sample path. (b) The α-skew Brownian motion sample path.

Just as standard Brownian motion may be obtained as the fine-scale limit (in distribution) of rescaled simple symmetric random walks, *c.f.,* Bhattacharya and Waymire (2009), the work of Harrison and Shepp (1981) showed that the $\alpha-$skew Brownian motion may be obtained in the fine-scale limit of simple random walks $S_n^{(\alpha)}, n \geq 0$, starting from 0, having displacement probabilities

$$P(S_{n+1}^{(\alpha)} - S_n^{(\alpha)} = 1 | S_n^{(\alpha)} = y) = P(S_{n+1}^{(\alpha)} - S_n^{(\alpha)} = -1 | S_n^{(\alpha)} = y) = \frac{1}{2}, \quad y \neq 0, n \geq 1 \quad (3.13)$$

and

$$P(S_{n+1}^{(\alpha)} - S_n^{(\alpha)} = 1 | S_n^{(\alpha)} = 0) = \alpha, \quad P(S_{n+1}^{(\alpha)} - S_n^{(\alpha)} = -1 | S_n^{(\alpha)} = 0) = 1 - \alpha, \quad n \geq 0 \quad (3.14)$$

This is precisely the discrete space-time stochastic particle motion independently introduced into the hydrology literature by Uffink (1985).

The stochastic particle position $\mathbf{Y}(t)$ at time t in three dimensions may be denoted $\mathbf{Y}(t) = (Y_1(t), Y_2(t), Y_3(t))$, where each coordinate defines a one-dimensional process. In the case where the interface is defined by $y_2 = 0$ (Fig 3.1a) parallel to the flow, the stochastic differential equation takes the form

$$\begin{aligned} dY_1(t) &= vdt + \sqrt{2D(Y_2(t))}\, dB_1(t) \\ dY_2(t) &= \sqrt{2D_T(Y_2(t))}\, dB^{(\alpha^*)}(t) \\ dY_3(t) &= \sqrt{2D_T(Y_2(t))}\, dB_3(t), \end{aligned} \tag{3.15}$$

where

$$\alpha^* = \frac{\sqrt{D^+}}{\sqrt{D^+} + \sqrt{D^-}}, \tag{3.16}$$

Here, $B_1(t)$ and $B_3(t)$ are independent one-dimensional standard Brownian motions, and $B^{(\alpha^*)}(t)$ is the appropriate skew Brownian motion (Ramirez et al., 2006). Notice that the interface is reflected in the structure of the coordinate process Y_2 in terms of a rescaled skew Brownian motion for a particular physically determined value of $\alpha = \alpha^*$. The corresponding transition probabilities of the Y_2 coordinate are given by the complex-looking, but nonetheless quite tractable, formulas Ramirez et al. (2006)

$$p^{(\alpha^*)}(y_0, y; t) = \begin{cases} \frac{1}{\sqrt{4\pi D^+ t}} \left[\exp\left\{ -\frac{(y-y_0)^2}{4D^+ t} \right\} + \frac{\sqrt{D^+}-\sqrt{D^-}}{\sqrt{D^-}+\sqrt{D^+}} \exp\left\{ -\frac{(y+y_0)^2}{4D^+ t} \right\} \right] \\ \qquad \text{if } y_0 > 0, y > 0 \\ \frac{1}{\sqrt{4\pi D^- t}} \left[\exp\left\{ -\frac{(y-y_0)^2}{4D^- t} \right\} - \frac{\sqrt{D^+}-\sqrt{D^-}}{\sqrt{D^-}+\sqrt{D^+}} \exp\left\{ -\frac{(y+y_0)^2}{4D^- t} \right\} \right] \\ \qquad \text{if } y_0 < 0, y < 0 \\ \frac{1}{\sqrt{D^+}+\sqrt{D^-}} \frac{1}{\sqrt{\pi t}} \exp\left\{ -\frac{(y\sqrt{D^-}-y_0\sqrt{D^+})^2}{4D^- D^+ t} \right\} & \text{if } y_0 \le 0, y > 0 \\ \frac{1}{\sqrt{D^+}+\sqrt{D^-}} \frac{1}{\sqrt{\pi t}} \exp\left\{ -\frac{(y\sqrt{D^+}-y_0\sqrt{D^-})^2}{4D^- D^+ t} \right\} & \text{if } y_0 \ge 0, y < 0. \end{cases} \tag{3.17}$$

In the case where the uniform velocity field is orthogonal to the plane defined by $y_1 = 0$ (Fig 3.1b), the particle motion involves the local time of the coordinate process Y_1

as follows:

$$dY_1(t) = \frac{D^+ - D^-}{D^+ + D^-} dL_t^0(Y_1) + v\,dt + \sqrt{2D(Y_1(t))}\,dB_1(t) \tag{3.18}$$

$$dY_2(t) = \sqrt{2D_T(Y_1(t))}\,dB_2(t) \tag{3.19}$$

$$dY_3(t) = \sqrt{2D_T(Y_1(t))}\,dB_3(t), \tag{3.20}$$

Here, B_1, B_2, B_3 are again independent one-dimensional standard Brownian motions, and we have made use of the the local time $L_t^0(Y_1)$. The simplest definition of local time at a point a is as a density for the amount of time the stochastic particle spends at that point; in other words,

$$L_t^a(Y_1) = \lim_{\epsilon \downarrow 0} \frac{1}{\epsilon} \int_0^t \mathbf{1}[a - \epsilon < Y_1(t') < a + \epsilon] 2D(Y_1(t'))dt' \tag{3.21}$$

Here the function $\mathbf{1}$ is an indicator function (which defined as being unity when the inequality is satisfied and zero ptherwise).

For $a \neq 0$ and ϵ small enough,

$$\mathbf{1}[a - \epsilon < Y_1(t') < a + \epsilon] 2D(Y_1(t')) = \mathbf{1}[a - \epsilon < Y_1(t') < a + \epsilon] 2D(a). \tag{3.22}$$

Prior to taking the small ϵ limit, the first integral term $\int_0^t \mathbf{1}[a - \epsilon < Y_1(t') < a + \epsilon]dt'$ measures the amount of time the particle spends between $a \pm \epsilon$ during interval of time 0 to t; this is called the *occupation time* (Γ_t) of the interval $a \pm \epsilon$. Dividing by ϵ and multiplying by the local dispersion coefficient $2D(a)$ defines the *local time* at a in the limit as $\epsilon \to 0$. Thus, in the case $a \neq 0$, one has formally

$$L_t^a(Y_1) = 2D(a) \int_{t'=0}^{t'=t} \delta(a - Y_1(t'))dt' \tag{3.23}$$

Note that the term "local time" is adopted because of a long-held convention in the literature; the units of the local time are the reciprocal of the units of the process being considered. In this case the local time has length units.

On the other hand, the interface at $y_1 = 0$ is shown to produce a nontrivial contribution to this local time at $a = 0$. Note that from (3.21),

$$L_t^0(Y_1) = 2D^- \lim_{\epsilon \downarrow 0} \frac{1}{\epsilon} \int_0^t \mathbf{1}[-\epsilon < Y_1(t') < 0]dt' + 2D^+ \lim_{\epsilon \downarrow 0} \frac{1}{\epsilon} \int_0^t \mathbf{1}[0 \leq Y_1(t') < \epsilon]dt' \quad (3.24)$$

The interface at $y_1 = 0$ has the effect that occupation tine of the process Y_1 of the interval $(-\epsilon, 0)$ and the interval $[0, \epsilon)$ are scaled differently. This different scaling gets reflected in the factor $\frac{D^+ - D^-}{D^+ + D^-}$ present in equation (3.18).

The presence of local time and drift in this case presents substantially new mathematical challenges for both Monte-Carlo numerical simulations and computation of the fundamental solution to the convection-dispersion equation or, equivalently, the transition probabilities of the particle motion process. In the next section, we describe how this is overcome by a mathematical transformation from a convection-dispersion to a related reaction-dispersion equation, where the concentration can then be explicitly computed via an exponential transformation and a fundamental expression from the theory of stochastic processes and partial differential equations known as the Feynman-Kac formula (*e.g.*, Bhattacharya and Waymire, 1990). Once this reaction-dispersion concentration is calculated, it is a simple matter to transform it back to the desired convective-dispersion concentration.

3.3 An Expected Value Formula for Concentration

As noted in the previous section, see Eq (3.18), the structure of the coordinate process $Y = Y_1$ across the interface is complicated by the effects of both drift and local time at zero. This is the focus of our analysis in this section. In particular we consider the system for which the flux is always aligned with the y_1-axis, and that the concentration field is uniform in the other two orthogonal directions (together, these imply that we have one-dimensional transport). The corresponding one-dimensional convection-dispersion equation takes the form

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial y}(D(y)\frac{\partial c}{\partial y}) - v\frac{\partial c}{\partial y} \tag{3.25}$$

$$c(0^+,t) = c(0^-,t), \qquad D^+\frac{\partial c}{\partial y}(0^+,t) = D^-\frac{\partial c}{\partial y}(0^-,t). \tag{3.26}$$

First, in regard to the interpretation of *local time*, note that we can apply the outer differential to the second order term of Eq (3.25) to yield what is frequently referred to as the Kolmogorov backward equation

$$\frac{\partial c}{\partial t} = (D(y)\frac{\partial^2 c}{\partial y^2}) - \left(v - (D^+ - D^-)\delta(y)\right)\frac{\partial c}{\partial y} \tag{3.27}$$

or, by a simple rearrangement of differentiated terms, the Kolmogorov forward (Fokker-Plank) equation

$$\frac{\partial c}{\partial t} = \frac{\partial^2}{\partial y^2}(D(y)c) - \frac{\partial}{\partial y}\left([v + (D^+ - D^-)\delta(y)]c\right) \tag{3.28}$$

In either case, the derivative of the dispersion coefficient generates a jump at the origin that contributes to the total convective flux. The local time may be viewed as the corresponding correction term that accounts for this additional convective flux at the discontinuity in the stochastic particle motion.

In regard to the presence of the velocity (drift) term in the analysis of the particle motions, our approach has been to transform this problem into one in which the drift term appears in the form of a reactive source. The first step in this regard is to define the transformation

$$\tilde{c}(y,t) = e^{-\frac{v}{2D(y)}y}c(y,t) \tag{3.29}$$

Then, it is straightforward to show that the quantity $\tilde{c}(y,t)$ evolves according to the reaction-dispersion equation

$$\frac{\partial \tilde{c}}{\partial t} = \frac{\partial}{\partial y}(D(y)\frac{\partial \tilde{c}}{\partial y}) - \frac{v^2}{4D(y)}\tilde{c} \tag{3.30}$$

$$\tilde{c}(0^+, t) = \tilde{c}(0^-, t), \qquad D^+\frac{\partial \tilde{c}}{\partial y}(0^+, t) = D^-\frac{\partial \tilde{c}}{\partial y}(0^-, t). \tag{3.31}$$

Moreover, from (3.29),

$$\tilde{c}(y, 0) = c(y, 0)e^{-\frac{v}{2D(y)}y}. \tag{3.32}$$

It follows from the Feynman-Kac formula that

$$c(y,t) = e^{\frac{v}{2D(y)}y}\tilde{c}(y,t) = e^{\frac{v}{2D(y)}y}\left\langle c_0(S^*(t))e^{-\frac{v}{2D(S^*(t))}S^*(t)} \exp\left\{-\int_0^t \frac{v^2}{4D(S^*(t'))}dt'\right\}\right\rangle \tag{3.33}$$

Here, the expectation operator is defined by

$$\langle g(U)\rangle = \int_{-\infty}^{\infty} uf(u)du \tag{3.34}$$

where $f(u)$ represents the pdf of the random variable $U = c_0(S^*(t)) \exp\left\{-\frac{v}{2D(S^*(t))}S^*(t)\right\}$ $\times \exp\left\{-\int_0^t \frac{v^2}{4D(S^*(t'))}dt'\right\}$. The term $S^*(t), t \geq 0$, denotes the rescaled (physical) skew Brownian motion started at y defined by

$$S^*(t) = \begin{cases} \sqrt{2D^+}B^{(\alpha^*)}(t) & \text{if} \quad B^{(\alpha^*)}(t) \geq 0 \\ \sqrt{2D^-}B^{(\alpha^*)}(t) & \text{if} \quad B^{(\alpha^*)}(t) < 0. \end{cases} \tag{3.35}$$

In view of the special form (3.7) of the dispersion coefficient, the formula (3.33) may be re-expressed in terms of the occupation time, Γ_t^+, measuring the amount of time before t that the α^* skew Brownian motion spends on the positive axis, as follows.

$$c(y,t) = e^{\frac{v}{2D(y)}y}e^{-\frac{v^2}{4D^-}t}\left\langle c_0(S^*(t))e^{-\frac{v}{2D(S^*(t))}S^*(t)} \exp\left\{-\frac{v^2}{4}(\frac{1}{D^+} - \frac{1}{D^-})\Gamma_t^+\right\}\right\rangle. \tag{3.36}$$

Now the computation of the indicated expected value in (3.33) can be re-expressed in terms of the joint probability distribution of the position $S^*(t)$ and the occupation time Γ_t^+ at time t, i.e., the bivariate distribution of $(S^*(t), \Gamma_t^+)$. That is, the indicated expectation in (3.36) is defined by

$$\left\langle g(S^*(t), \Gamma_t^+) \right\rangle = \int\limits_0^\infty \int\limits_{-\infty}^\infty g(b,\tau) f(y; b, \tau) db d\tau \tag{3.37}$$

where, for fixed injection site y, the random variables $S^*(t)$ started at y, and Γ_t^+ have a bivariate pdf $f_{S_t^*, \Gamma_t^+}(y; b, \tau)$, with y as a parameter, determined at (3.43) below, and $g(b,\tau) = c_0(b) e^{-\frac{v}{2D(b)}b} \exp\left\{-\frac{v^2}{4}(\frac{1}{D^+} - \frac{1}{D^-})\tau\right\}$.

In a more comprehensive mathematical treatment by Appuhamillage et al. (2011b), the trivariate distribution of $(B_t^{(\alpha)}, L_t^0, \Gamma_t^+)$ is computed. In particular it is shown that for $x \geq 0,\ b > 0,\ \ell > 0,\ 0 < \tau < t$, one has

$$\begin{aligned} &P_x\left(B_t^{(\alpha)} \in db, L_t^0 \in d\ell, \Gamma_t^{(\alpha)} \in d\tau\right) \\ &\quad = 2(1-\alpha) h\left(\tau; \alpha\ell + x\right) h\left(t - \tau; (1-\alpha)\ell - b\right) db d\ell d\tau \end{aligned} \tag{3.38}$$

where $h\left(s; r\right) ds = P_r\left(T^{(\alpha)} \in ds\right)$ is the distribution of the first time for skew Brownian motion to reach zero starting from r. Since this coincides with that of standard Brownian motion it follows that

$$h(s;r)ds = P_r\left(T^{(\alpha)} \in ds\right) = \frac{|r|}{\sqrt{2\pi s^3}} \exp\left\{-\frac{r^2}{2s}\right\} ds; \quad s > 0 \tag{3.39}$$

It is also shown for $x < 0,\ b > 0,\ 0 < \tau < t$,

$$\begin{aligned} &P_x\left(B_t^{(\alpha)} \in db, L_t^0 \in dl, \Gamma_t^+ \in d\tau\right) \\ &\quad = 2\alpha h\left(t - \tau; (1-\alpha)\ell\right) h\left(\tau; \alpha\ell + b + x\right) db d\ell d\tau. \end{aligned} \tag{3.40}$$

From this one may derive the bivariate distribution of $(B_t^{(\alpha)}, \Gamma_t^+)$ by integrating over $\ell > 0$. For the application at hand we assume injections at $b < 0$ and breakthrough at $y > 0$.

It is convenient to define A, B and C^2 by $A = \frac{\alpha y(t-\tau)-(1-\alpha)b\tau}{\alpha^2(t-\tau)+(1-\alpha)^2\tau}$, $B = \frac{\alpha^2(t-\tau)+(1-\alpha)^2\tau}{2\tau(t-\tau)}$, and $C^2 = \frac{y^2(t-\tau)+b^2\tau}{\alpha^2(t-\tau)+(1-\alpha)^2\tau}$. With this notation direct calculations shows that the probability density of the distribution of $(B_t^{(\alpha)}, \Gamma_t^+)$ is given by

$$\begin{aligned} f_{B_t^{(\alpha^*)},\Gamma_t^+}(y;b,\tau)dbd\tau &= P_y\left(B_t^{(\alpha)} \in db, \Gamma_t^+ \in d\tau\right) \\ &= \left[\int_0^\infty 2(1-\alpha)h\left(\tau;\alpha\ell+x\right)h\left(t-\tau;(1-\alpha)\ell-b\right)d\ell\right]dbd\tau \\ &= \frac{(1-\alpha)}{\pi\sqrt{\tau(t-\tau)}}\left[\frac{(1-\alpha)^3\tau y-\alpha^3(t-\tau)b}{\left[\alpha^2(t-\tau)+(1-\alpha)^2\tau\right]^2}\exp(-BC^2)\right. \qquad (3.41) \\ &\left. + \frac{\alpha(1-\alpha)}{\left[\alpha^2(t-\tau)+(1-\alpha)^2\tau\right]}\frac{\sqrt{\pi}}{2\sqrt{B}}\mathrm{erfc}(A\sqrt{B})\left[1-2B(C^2-A^2)\right]\exp(-B(C^2-A^2))\right]. \end{aligned}$$

where erfc(u) is the complementary Gauss error function defined as

$$\mathrm{erfc}(u) = \frac{2}{\sqrt{\pi}}\int_u^\infty e^{-x^2}dx. \qquad (3.42)$$

From this bivariate density one may then compute the expected value in (3.36) as follows. From (3.41), define

$$f_{S_t^*,\Gamma_t^+}(y;b,\tau) = \frac{1}{\sqrt{2D(b)}}f_{B_t^{(\alpha^*)},\Gamma_t^+}\Big(\frac{y}{\sqrt{2D(y)}};\frac{b}{\sqrt{2D(b)}},\tau\Big). \qquad (3.43)$$

Then it follows that (3.36) may be expressed as

$$\begin{aligned} c(y,t) = &\exp\Big\{\frac{v}{2D(y)}y - \frac{v^2}{4D^-}t\Big\}\int_0^t\int_{-\infty}^\infty c_0(b)\exp\Big\{-\frac{v}{2D(b)}b\Big\}\exp\Big\{-\frac{v^2}{4}(\frac{1}{D^+}-\frac{1}{D^-})\tau\Big\} \\ &\cdot\frac{1}{\sqrt{2D(b)}}f_{B^{(\alpha^*)},\Gamma_t^+}\Big(\frac{y}{\sqrt{2D(y)}};\frac{b}{\sqrt{D(b)}},\tau\Big)\,db\,d\tau \qquad (3.44) \end{aligned}$$

Here $c_0(b)$ denotes the initial concentration field. Taking $c_0(b) = \delta_{-L}(b)$ yields the fundamental solution as an important special case. While these explicit formulae for the concentration are algebraically somewhat complicated expressions, even compared to the formula for the parallel interface given by Eq (3.17), they nonetheless involve only well-known algebraic and transendental functions. Thus it is relatively straightforward to construct plots of concentration and flux-averaged breakthrough formulae. These are provided in the next section.

In closing this section we note that as the conservation law for the flux-averaged breakthrough must hold, one may derive it from the the theory by simply integrating the convection-dispersion equation as follows for $L > 0$, and total initial mass c_0. Specifically,

$$c_0/v = \frac{1}{v}\int_0^\infty \int_{-\infty}^L \frac{\partial c}{\partial t} dydt = \frac{1}{v}\int_0^\infty \{D^+ \frac{\partial c}{\partial y}(L,t) - vc(L,t)\}dt = \int_0^\infty c_f(t)dt. \quad (3.45)$$

Apart from its physical significance, this is also a useful observation in assessing the breakthrough plots.

3.4 Breakthrough Curve Symmetries: Resident versus Flux-averaged Concentrations

There is a rather large body of work in the hydrology literature that has examined the role of measurement in the interpretation of experiments. The goal of this section is to apply the previous mathematical development to analyze the symmetries and asymmetries in the breakthrough curves as measured by (1) the resident concentration and (2) the flux-averaged concentration. Both mass and molar units can be used to measure these quantities, but we will adopt the mass perspective here. Although the differences between the resident and flux-averaged concentrations have been identified in the literature (Kreft and Zuber, 1978; Van Genuchten and Parker, 1984; Parker and Van Genuchten, 1984), to date they have been discussed only infrequently and incompletely. Previous work (*e.g.*,Kreft and Zuber (1978)) focused exclusively on one-dimensional systems and have assumed that the measurement process is ideal (*i.e.*, spatially and temporally infinitesimal). Generalizing these previous definitions, one can propose the following for the generalized resident mass concentration and mass flux.

$$\bar{c}(y,t) = \int_{t'=-\frac{1}{2}\Delta t}^{t'=\frac{1}{2}\Delta t} \int_{x\in\Omega(y)} c(y-x, t-t') m_1(x,t') dt' dx \tag{3.46}$$

$$\bar{\mathcal{J}}(y,t) = \int_{t'=-\frac{1}{2}\Delta t}^{t'=\frac{1}{2}\Delta t} \int_{x\in A(y)} \mathcal{J}(y-x, t-t') m_2(x,t') dt' dx \tag{3.47}$$

Here, m_1 and m_2 represent instrument response (or instrument weighting) functions, as described by Baveye and Sposito (1984) and Cushman (1984). In these expressions, y is the location for a reference volume (the support of m_1 or m_2) and $\mathcal{J}$ is the total mass flux. In the conventional treatments of the resident and flux-averaged concentrations, the weighting functions are taken to be

$$m_1(x,t') = \delta(x-y)\delta(t'-t) \tag{3.48}$$

$$m_2(x,t') = \delta(x-y) \tag{3.49}$$

For the resident concentration, this weighting function is an area averaged concentration in the physical system; in the 1-dimensional system, this yields immediately that $\bar{c}(y,t) = c(y,t) \equiv c_r(y,t)$. Here we have adopted the notation $c_r(y,t)$ to indicate the conventional definition of the resident concentration for 1-dimensional systems (*c.f.* Kreft and Zuber (1978); Van Genuchten and Parker (1984); Parker and Van Genuchten (1984)). For the flux-averaged concentration, it is easiest to consider the following limit process. For a finite time interval Δt, the mass that crosses a plane located at $y = L$ is given by

$$M(L,t,\Delta t) = \bar{\mathcal{J}}\Delta t \tag{3.50}$$

The total amount of fluid that crosses the same plane in Δt is

$$V(L,\Delta t) = v\Delta t \tag{3.51}$$

The flux-averaged concentration is then defined by

$$c_f(L,t) \equiv \lim_{\Delta t \to 0} \frac{M(L,t,\Delta t)}{V(L,\Delta t)} = \lim_{\Delta t \to 0} \frac{\bar{\mathcal{J}}(y,t)}{v} \tag{3.52}$$

Substituting Eqs (3.47), (3.49), (3.51), and (3.50) yields the definition for the flux-averaged concentration

$$c_f(L,t) = \frac{\mathcal{J}(L,t)}{v} \tag{3.53}$$

It is interesting to note that measurement conducted in the laboratory occur over finite (but not differential) time and space intervals. Therefore, the δ-function approximation of the instrument weighting functions is incorrect for any real measurement, and the error involved in this approximation will depend strongly upon the physical conditions of the experiment (*e.g.*, the Péclet number), and on the details of the particular instruments and methods used to measure the concentration. In any event, concentrations measured in the laboratory are generally not the resident or the flux-averaged concentration, but rather a more complex convolution in time and space that results in a concentration that has characteristic of both c_r and c_f.

3.4.1 Application of the Theory

As mentioned in the introduction, some recent experiments conducted by Berkowitz et al. (2009) have provided additional motivation for development of the results reported here. These experiments focussed on solute transport in a discontinuous medium that was structured essentially as illustrated in Fig 3.1b, where the mean velocity vector is assumed to be positive to the right. Three different uniform velocities were examined by Berkowitz et al. (2009), and for each velocity the experiment was conducted in both the fine-to-coarse and coarse-to-fine configurations (for a total of six different experimental configurations); the parameters associated with each of these six experiments are given in Table 3.1. The inlet boundary conditions was such that a constant total mass was injected in each of their experiments. The inlet boundary was located at $L = -20\ cm$, and the effluent (observation) boundary at $L = 20\ cm$. Using our notation, the two configurations (fine-to-coarse and coarse-to-fine) examined for each velocity can be expressed by

$$\text{(coarse to fine):} \quad D(\mathbf{y}) = \begin{cases} D^- = D_{\text{coarse}} & \text{if} \quad y_1 < 0. \\ D^+ = D_{\text{fine}} & \text{if} \quad y_1 \geq 0 \end{cases} \tag{3.54}$$

$$\text{(fine to coarse):} \quad D(\mathbf{y}) = \begin{cases} D^- = D_{\text{fine}} & \text{if} \quad y_1 < 0. \\ D^+ = D_{\text{coarse}} & \text{if} \quad y_1 \geq 0 \end{cases} \tag{3.55}$$

With these definitions, the analytical solution given by Eq (3.44) was used to generate the solutions for the parameters sets specified in Table 3.1 as follows.

Experiment	v (cm/min)	D^+ (cm^2/min)	D^-(cm^2/min)	T (min)
1	0.448	0.430	0.0582	1.5
2	0.448	0.0582	0.430	1.5
3	0.179	0.172	0.0233	3.75
4	0.179	0.0233	0.172	3.75
5	0.134	0.129	0.0174	5.0
6	0.134	0.0174	0.129	5.0

TABLE 3.1: Parameter sets associated with the experiments conducted by Berkowitz et al. (2009).

First, values for v, D^+, and D^- for each of the six cases were used to generate the fundamental solution to Eqs (3.25)-(3.26) assuming that the initial condition was specified by $c(x, 0) = m_0\delta(-L)$, where m_0 indicates the initial mass injected into the system (Fig 3.3).

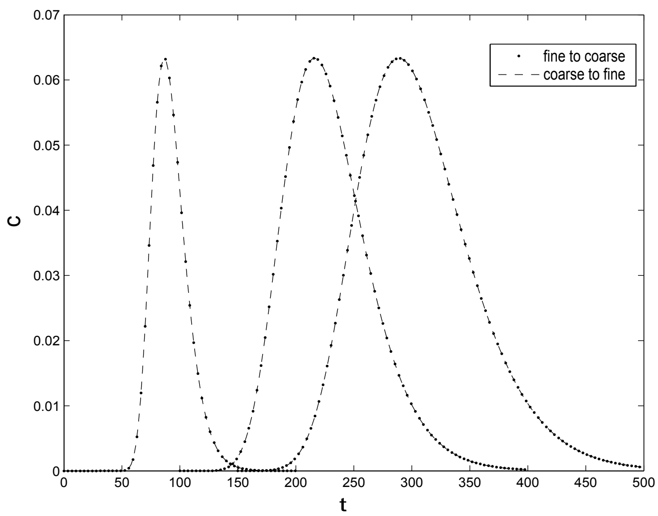

FIGURE 3.3: (a) Resident concentration breakthrough curves for a delta input at $L = -20\ cm$ and observation at $L = 20\ cm$. The physical set up is as illustrated in Fig 3.1.

The experiments conducted by Berkowitz et al. (2009) were intended to explore the breakthrough curves in the presence of the two different configurations (fine-to-coarse and coarse-to-fine). The measured concentration reported by Berkowitz et al. (2009) could be most closely interpreted as the flux-averaged one [B. Berkowitz, personal communication], c_f, although, as indicated above, experimental measurements generally do not represent exactly the flux-averaged or the resident concentration. Because the purpose of these experiments was primarily to analyze the properties of the breakthrough under mirror symmetric flow conditions, the concentration measurement technique was not calibrated to give explicit values of measured concentration, and the time that injection was started for each experiment was not recorded. Thus, it is not generally possible to directly model the results reported in Berkowitz et al. (2009) without free parameters. In the results reported below, we have adopted conditions similar to the experiments reported by Berkowitz et al. (2009) (as represented in Table 3.1) in order to analyze the same qualitative features, but no direct comparison with their data is attempted because of experimental limitations.

3.4.2 Resident Concentration

The first mathematical symmetry phenomena that is interesting to note is that found in the case of skew Brownian motion and physical skew diffusion particle motions obtained by Ramirez et al. (2008). When there is no convection, one may observe in Eq (3.12) that, although the transition probabilities of the standard skew Brownian motion itself are not spatially symmetric for $\alpha \neq \frac{1}{2}$, the value $\alpha^* = \frac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}$ together with the respective rescalings defined by $\sqrt{2D^{\pm}}$, makes the transition probabilities given by Eq (3.17) of the actual physical skew diffusion process spatially symmetric. As a result, the breakthrough of resident concentration is (temporally) symmetric with respect to the coarse-fine and fine-coarse mirror symmetries (assuming that the injection is at $x = -L$ and that the observation is made at $x = L$). In other words, as would be expected the physical processes lead to a symmetrization in the parameterization of the standardized skew Brownian motion. A mathematical proof of this symmetry may be derived from the pdf (3.17) by simply taking $y_0 = -L$ and $y = L > 0$ and note the invariance in the resulting function of time under an exchange of D^+ and D^- in the third line of the display.

The same symmetry of the breakthrough resident concentration curve as depicted in Fig 3.4 also follows mathematically in the presence of convection across the interface. This symmetry agrees with that reported by Berkowitz et al. (2009) based on numerical simulations of Fickian advection-dispersion conducted separately from their experiments. Note that here, for consistency with the work of Berkowitz et al. (2009), we have non-dimensionalized the transport equations to be of the form

$$\frac{\partial c_r}{\partial t^*} = -\frac{\partial c_r}{\partial \xi} + \frac{1}{Pe^{\pm}}\frac{\partial^2 c_r}{\partial \xi^2} \tag{3.56}$$

where here t^* is the nondimensional time, often referred to as pore volumes (PV), given by $t^* = tv/L$, and $Pe^{\pm}$ are the non-dimensional Péclet numbers, given by $Pe^- = (vL)/D^-$ and $Pe^+ = (vL)/D^+$, respectively.

The mathematical argument regarding the symmetry in the effluent concentration as a function of the configuration is essentially the same as above, but now one must consider the bivariate density in Eq (3.41). Although tedious, it nonetheless follows that the symmetry property described above persists even in the presence of convection, so that the resident concentration at $x = L$ is insensitive to the choice of configuration (fine-to-coarse or coarse-to-fine). Note that this statement is not generally true for any other observation location. The symmetry is due, in part, to the symmetry in the physical configuration; if the coarse and fine segments of the one-dimensional system were not of identical length, then the fine-to-coarse versus coarse-to-fine symmetry would no longer hold in general.

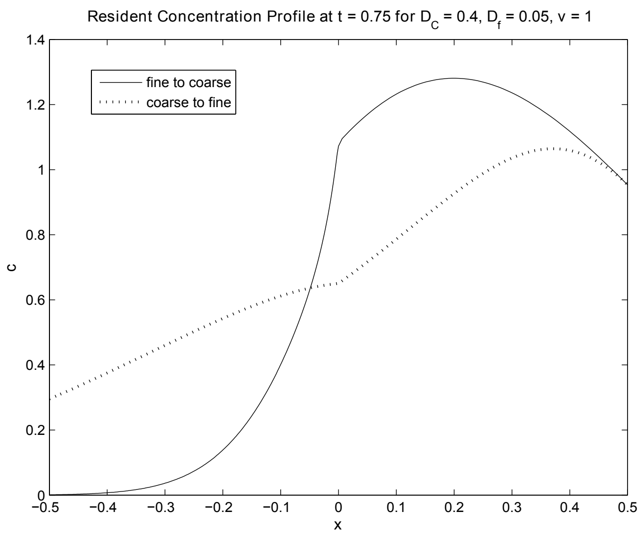

FIGURE 3.4: The spatial distribution of the resident concentration. The curves here are non-dimensionalized following Berkowitz et al. (2009). For the case where the interface is located exactly half-way along the column, the analytical solution presented in Eq (3.44) is the same regardless of the configuration (i.e., fine-to-coarse and coarse-to-fine yield the same solutions). Notably, the same result is not true for the flux-averaged concentration, c_f.

3.4.3 Flux-Averaged Concentration

From the developments above, the flux-averaged breakthrough at the effluent ($y = L$) is defined through the flux, $J = vc_r - D(y)\partial c_r/\partial y$, by Eq (3.53)

$$c_f(L,t) = c_r(L,t) - \frac{D(L)}{v}\left.\frac{\partial c_r}{\partial y}\right|_{L,t} \tag{3.57}$$

Plots of the flux-averaged breakthrough curves computed above are depicted in the figures below; see Fig 3.5a. In Fig 3.5b we have also plotted the flux-averaged concentration normalized so that the area under the breakthrough curve represents the total mass injected into the system. Because the total mass injected for each of the six experiments identified in Table 3.1 is constant, this particular representation makes it easier to see how changing the Péclet number and the configuration influences the resulting breakthrough curve properties relative to the other experiments.

The asymmetry properties in the flux-averaged breakthrough curve discovered in the experiments of Berkowitz et al. (2009) on a change in configuration from fine-to-coarse and coarse-to-fine may also be mathematically derived from the Fickian convective-dispersive equations. To compute these curves from the formulae derived here one first takes $c_0(b) = \delta_{-L}(b)$ to obtain the fundamental solution $g(-L, y, t)$ from (3.44). Duhamel's principle can then be applied to obtain a formula for the resident concentration corresponding to an injection at the point $-L$ over an arbitrary time interval $0 \leq t \leq T$; see Bhattacharya and Waymire (2009). Specifically, denote the rate at time t at which mass in injected at the point $b = -L$ by $q_{\text{inj}}(t)$. Using Duhamel's principle one has for zero initial concentration that

$$c(y,t) = \int_0^t q_{\text{inj}}(s) g(-L, y, t-s) ds. \tag{3.58}$$

One may observe that as a consequence of (3.58), and since the integrand is symmetric under a change of coarse-to-fine versus fine-to-coarse configurations, the resident concentration at $y = L$ remains symmetric for time dependent injections too. Also, from the expression in (3.58) for the resident concentration, the flux-averaged concentration can be computed directly by using the relation given in Eq (3.57). Essentially, this requires only that one first compute the spatial derivative given by

$$\begin{aligned}\frac{\partial}{\partial y} f_{B_t^{(\alpha^*)},\Gamma_t^+}(y;b,\tau)dbd\tau = {} & \frac{\alpha(1-\alpha)^2}{\pi\sqrt{\tau(t-\tau)}}\frac{1}{\alpha^2(t-\tau)+(1-\alpha)^2\tau} \\ & .\Big\{\Big[1-\frac{2(1-\alpha)[(1-\alpha)y+\alpha b]}{\alpha^2(t-\tau)+(1-\alpha)^2\tau}\Big] \\ & \quad -\frac{2(1-\alpha)[(1-\alpha)y+\alpha b]}{\alpha^2(t-\tau)+(1-\alpha)^2\tau}[1-2B(C^2-A^2)]\Big\} \qquad (3.59)\\ & .\exp(-B(C^2-A^2))\frac{\sqrt{\pi}}{2\sqrt{B}}\mathrm{erfc}(A\sqrt{B}) \\ & -\frac{\alpha^2(1-\alpha)^2}{\pi\sqrt{\tau(t-\tau)}}\frac{1}{[\alpha^2(t-\tau)+(1-\alpha)^2\tau]^2}\frac{\alpha}{2\tau B}[1-2B(C^2-A^2)] \\ & .\exp(-B(C^2-A^2))\exp(-BA^2) \qquad (3.60)\\ & +\frac{(1-\alpha)^4}{\pi\sqrt{\tau(t-\tau)}}\frac{\tau}{[\alpha^2(t-\tau)+(1-\alpha)^2\tau]^2}\exp(-BC^2) \\ & +\frac{(1-\alpha)}{\pi\sqrt{\tau(t-\tau)}}\frac{y}{\tau B}\frac{\alpha^3(t-\tau)b-(1-\alpha)^3\tau b}{\alpha^2(t-\tau)+(1-\alpha)^2\tau}\exp(-BC^2)\end{aligned}$$

In view of the symmetry in the breakthrough resident concentration noted above, it follows that the asymmetry depicted in the plots of the flux-averaged breakthrough results from an asymmetry in the dispersive flux, $d(L) = -D(L)\frac{\partial c}{\partial y}\mid_L$ under the exchange of $\sqrt{D^+}$ and $\sqrt{D^-}$ for an injection at $y = -L$ and breakthrough at $y = L > 0$. This is most easily seen in the resulting breakthrough curves computed from this solution rather than the solution itself. In Fig 3.5, the differences among the flux-averaged breakthrough curves upon changing the configuration is evident. In particular, one can note that in each case, the time to the peak flux-averaged concentration for the coarse-to-fine configuration is greater than for the fine-to-coarse configuration.

This result can be explained by the dependance of the flux-averaged concentration

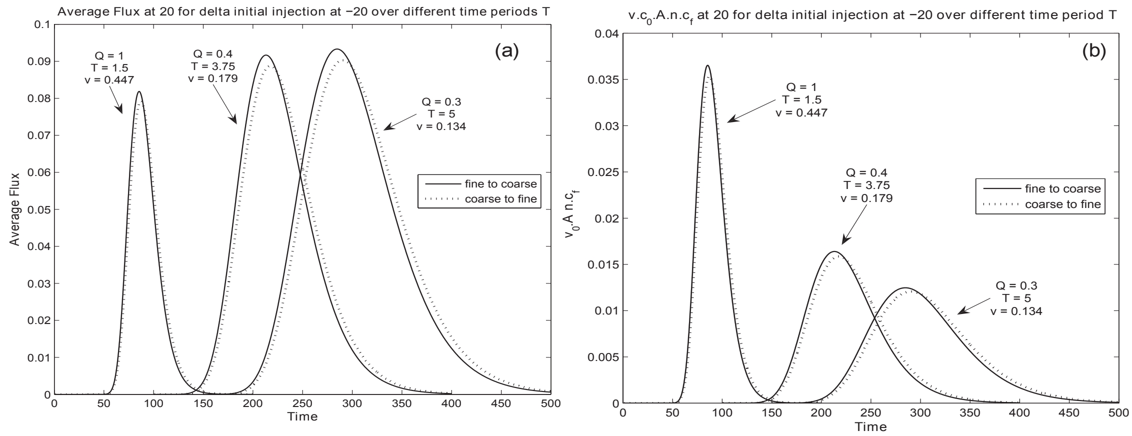

FIGURE 3.5: Plots of (a) the flux-averaged concentration for the six models identified in Table 1. (b) The same plots, but normalized so that the areas underneath the curves represent the total (constant) mass injected.

upon the local gradients in the resident concentration. The flux-averaged concentration depends upon the spatial derivatives of $c(y,t)$. For the case of a discontinuous medium, this means that the concentration at the interface depends upon both $\partial c_r/\partial y|_{I^-,t}$ and $\partial c_r/\partial y|_{I^+,t}$, as indicated by Eq (3.3). However, these gradients evolve differently in the coarse and fine media. This means that at the interface, the gradients of the concentration do depend upon the configuration (fine-to-coarse versus coarse-to-fine), and this dependency essentially breaks the symmetry that can be observed for the breakthrough curve of the resident concentration.

In our results, the differences between the coarse-to-fine and fine-to-coarse configurations are not as large as those reported by Berkowitz et al. (2009). There are several possible reasons for this discrepancy. First, the theory assumes a perfect interface. It is possible that at the discontinuity imperfections in the interface and local ordering of particles may actually increase the measured rate of spreading. Secondly, the theory has been developed for an infinite system rather than a finite one. The influence of the boundary conditions may in fact be significant enough that the infinite-field approximation is not adequate. Each of these can be checked through careful experimental controls.

3.5 Summary and Future Directions

The main point of this paper is to precisely determine the structure of concentration and breakthrough curves as predicted by Fickian convection-dispersion conservation laws in the presence of a sharp interface orthogonal to the flow direction. The theory exhibits the general qualitative symmetric and asymmetric features of concentration and breakthrough predicted by experiment. Although our solutions do not replicate the experimental breakthrough curve values for the coarse-to-fine and fine-to-coarse configurations as large as those found by Berkowitz et al. (2009), they do provide compelling evidence that the observed symmetries and asymmetries can be explained by the dynamics of the transport process in the vicinity of the discontinuous interface using the deterministic Fickian conservation laws. More carefully controlled experiments should help to clarify the issue of more precisely replicating measured values.

A number of interesting directions are suggested by this work. Having resolved the principal coordinate directions, it will be natural to pursue applications to more complicated geometries. The solution provided here also provides a benchmark to test various possible numerical and/or Monte-Carlo particle tracking schemes designed to address interfacial discontinuities. The role of local time presents one of the biggest challenges to Monte-Carlo simulation of particle tracking schemes. An attempt is given in Lejay (2008) to eliminate it by first making a transformation to remove the drift different from that used here. Their transformation removes the drift but introduces a coefficient $\rho(x)$ of the second order term that is required to be a bounded function. Unfortunately, if this is applied to the problem at hand, i.e., Eq (3.25), the resulting $\rho(x)$ is unbounded, in fact, exhibits exponential growth.

An alternative way in which to quantify the asymmetry in breakthrough is in terms of the so-called first passage time of injected particles at $-y$ to reach the removal point at

y. For an arrangement of injection in the fine region and removal in the coarse region or vice versa, one may ask the question "in which configuration would particles be removed first?" It is shown by Appuhamillage et al. (2011b) that the fine-to-coarse first passage time is stochastically larger than the coarse-to-fine first passage time. This implies that the mean breakthrough time is larger in a fine-to- coarse arrangement than in a coarse-to-fine arrangement. However, this analysis has been made without explicit computation of the first passage time density [Appuhamillage et al. (2011b)]. The determination of the first passage time density has recently been obtained for skew Brownian motion (without drift) by T. A. Appuhamillage and D. Sheldon (First passage time of skew Brownian motion, manuscript in preparation, 2010); however, comparisons with the flux-averaged breakthrough curves have not been done yet.

Acknowledgments

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3.6 Asymmetries in Occupation Times

In the second chapter of this thesis, we saw the asymmetries in first passage times of skew Brownian motion. It is not hard to show similar results in the first passage times of skew diffusion. In this chapter we saw the same asymmetry in flux average breakthrough curves, the physical quantity that can be thought mathematically as the first passage time.

Just as the first passage time of a process, the occupation time also plays a vital role when modeling natural phenomena. Suppose we want to model animal movement between a clearcut and a forested area using a diffusion model. Clearly their diffusion rates are different inside the forest and in the clearcut. If the animal is in danger in the clearcut region, it should move faster in there and hence has a higher diffusion rate in the clearcut. If the animal is in danger in the clearcut it should also occupy less time in there. This suggests that the animal has an effect at the interface between clearcut and the forest. The condition one may have at the interface in animal movement model is highly correlated with the animal's preference to occupy less time in one area compared to the other. In this section, we describe the effect of the interface condition on occupation time of underlying stochastic process.

There are two different occupation times defined in literature, one that defines using quadratic variation of the process and one without. The latter is the most useful one in models describing physical phenomena. Our results in this section are for occupation times of the second type. Let us first define the occupation time of a process X on the positive and negative real lines respectively as follows:

$$\widetilde{\Gamma}_{+}^{X}(t,\omega) = \int_0^t \mathbb{I}_{[X_s(\omega)>0]} ds$$
$$\widetilde{\Gamma}_{-}^{X}(t,\omega) = \int_0^t \mathbb{I}_{[X_s(\omega)<0]} ds$$

Let us consider a general one dimensional diffusion problem as follows:

$$\begin{aligned} \frac{\partial c}{\partial t} &= \frac{1}{2}\frac{\partial}{\partial x}\Big(\mathbf{D}(x)\frac{\partial c}{\partial x}\Big) \\ \mu\frac{\partial c}{\partial x}|_{0^+} &= (1-\mu)\frac{\partial c}{\partial x}|_{0^-} \\ c(t,0^+) &= c(t,0^-) \end{aligned} \tag{3.61}$$

where $\mathbf{D}(x) = D^{-}\mathbb{I}_{[x<0]} + D^{+}\mathbb{I}_{[x\geq 0]}$ and $0 \leq \mu \leq 1$.

Now assume X is the stochastic process associated with the equation and interface conditions (3.61). Then we have the following theorem.

Theorem 3.6.1. *Suppose $D^+ > D^-$. Then we have*

i. $\widetilde{\Gamma}^X_+(t,\omega) > \widetilde{\Gamma}^X_-(t,\omega)$ *if* $\mu > \dfrac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}$

ii. $\widetilde{\Gamma}^X_+(t,\omega) = \widetilde{\Gamma}^X_-(t,\omega)$ *if* $\mu = \dfrac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}$

iii. $\widetilde{\Gamma}^X_+(t,\omega) < \widetilde{\Gamma}^X_-(t,\omega)$ *if* $\mu < \dfrac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}$

Before proving the theorem let us consider the following change of variable for the equation (3.61). Define $\mu(x)$ by

$$\mu(x) = \begin{cases} 2\mu & \text{if } \; x > 0 \\ 2(1-\mu) & \text{if } \; x < 0. \end{cases} \tag{3.62}$$

Then for $u(t,x) = c(t,\mu(x)x)$, equations (3.61) becomes,

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{1}{2}\frac{\partial}{\partial x}\Big(\frac{\mathbf{D}(x)}{\mu^2(x)}\frac{\partial u}{\partial x}\Big) \\ \frac{\partial u}{\partial x}|_{0^+} &= \frac{\partial u}{\partial x}|_{0^-} \\ c(t,0^+) &= c(t,0^-) \end{aligned} \tag{3.63}$$

Suppose Y be the stochastic process associated with equations in (3.63). Then we have that $Y = \dfrac{X}{\mu(x)}$.

Now we are ready to prove our theorem.

Proof. The proof of this theorem uses the random time change describe later in Section 4.3.

Define $\varphi(x) = \frac{\mathbf{D}(x)}{\mu^2(x)}$. For each $t \geq 0$ and $\omega \in \Omega$, define a stopping time $\tau_\varphi(t,\omega)$ such that

$$\int_0^{\tau_\varphi(t,\omega)} \frac{1}{\varphi(B(s,\omega))} ds = t.$$

Again define S_φ such that $B(t, S_\varphi(\omega)) = B(\tau_\varphi(t,\omega),\omega) = Y(t,\omega)$. Then by the definition of $\widetilde{\Gamma}^X_+(t,\omega)$ we have,

$$\begin{aligned}\widetilde{\Gamma}^X_+(t,\omega) &= \int_0^t \mathbb{I}_{[X_s>0]}ds \\ &= \int_0^t \mathbb{I}_{[Y_s>0]}ds \\ &= \int_0^t \mathbb{I}_{[B(\tau_\varphi(s,\omega),\omega)>0]}ds \\ &= \frac{4\mu^2}{D^+}\int_0^{\tau_\varphi(t,\omega)} \mathbb{I}_{[B(s\prime,\omega)>0]}ds' \\ &= \frac{4\mu^2}{D^+}\widetilde{\Gamma}^B_+(\tau_\varphi(t,\omega))\end{aligned}$$

Similarly

$$\widetilde{\Gamma}^X_-(t,\omega) = \frac{4(1-\mu)^2}{D^-}\widetilde{\Gamma}^B_-(\tau_\varphi(t,\omega))$$

for a Brownian motion starting at 0.

Since $\widetilde{\Gamma}^B_+(t,\omega) = \widetilde{\Gamma}^B_-(t,\omega)$ for a Brownian motion starting at 0, we have the following relationship between occupation times of the process X.

$$\frac{D^-}{(1-\mu)^2}\widetilde{\Gamma}^X_-(t,\omega) = \frac{D^+}{\mu^2}\widetilde{\Gamma}^X_+(t,\omega). \tag{3.64}$$

The proof of the theorem follows from the the equation (3.64). □

Going back to our example described earlier, if we assume an animal occupies less time in the clearcut region, where it has higher diffusion rate, this theorem suggests that the interface condition one may consider in the model should not be the continuity of flux across the interface.

4 INTERFACES OF GENERAL GEOMETRIES

4.1 Introduction

In the second chapter of the thesis we analyzed the dispersion equation with piecewise constant dispersion coefficient and a constant drift with the addition of interface condition at places where the dispersion has jumps. In there we used the continuity of flux as the interface condition. Also the considered dispersion coefficient has jumps on a plane so that the interface is planar. We computed the transition probability density function of the underlying stochastic process which we referred in the chapter as skew diffusion with drift. This was an extension of the previous work of Ramirez et al. (2006) where they analyzed the no-drift case. In the third chapter we used the results from the second chapter to analyze breakthrough curves and occupation times of a solute when the solute is transported across an interface. Here again the interfaces we considered are planar.

In models describing natural phenomena one would often encounter interfaces which have more general geometries than planes. The specific nature or the condition at the interface can vary, depending on the specific phenomena. In the solute transport models discussed in chapter two and three (Fickean dispersion model), the interface condition is the continuity of flux. In models that capture the upwelling and downwelling phenomena in the ocean, for an example quasi geographic balance - hydrostatic approximation, typical interface condition is the continuity of derivatives across the interface; see Matano and Palma (2008). Also a more general interface condition can be found in heat transfer models in composite materials. i.e. $\lambda \nabla c \cdot \eta|_{+} = (1-\lambda)\nabla c \cdot \eta|_{-}$, where η is a unit normal to the interface, $0 \leq \lambda \leq 1$ and $\pm$ represent the two regions separated by the interface; see Carslaw and Yeager (1959). In all the cases they assume that the unknown function is continuous across the interface.

In this chapter we consider interfaces that are graphs of functions. The PDE's we consider here are convection reaction-diffusion equations with the interface condition being the general interface condition described in the previous paragraph.

To introduce the problem, let g be a real valued C^2 function on $\mathbb{R}^{n-1}$. Denote the graph of g by $\mathcal{S} = \{(x_1, x_2, ..., x_n) \in \mathbb{R}^n | x_n = g(x_1, x_2, ..., x_{n-1})\}$. Now denote the two regions separated by $\mathcal{S}$ by $\mathcal{A}_1 = \{(x_1, x_2, ..., x_n) \in \mathbb{R}^n \mid x_n > g_1(x_1, x_2, ..., x_{n-1})\}$ and $\mathcal{A}_2 = \{(x_1, x_2, ..., x_n) \in \mathbb{R}^n \mid x_n < g_1(x_1, x_2, ..., x_{n-1})\}$.

For a real valued function $c \in C([0,\infty), \mathbb{R}^n) \cap C^{1,2}([0,\infty), \mathcal{A}_1 \cup \mathcal{A}_2)$, we consider the convection reaction-diffusion equation

$$\frac{\partial c}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{v}c) = \frac{1}{2}\nabla_{\mathbf{x}} \cdot (\mathbf{D}(\mathbf{x})\nabla_{\mathbf{x}} c) + R(\mathbf{x})c \quad t \geq 0, \quad \mathbf{x} \in \mathbb{R}^n \setminus \mathcal{S} \tag{4.1}$$

with the initial condition $c(0, \mathbf{x}) = c_0(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^n$.

In the PDE (4.1), we have following assumptions:

[A1 :] The diffusion coefficient $\mathbf{D}$ is piecewise constant on each $\mathcal{A}_1$ and $\mathcal{A}_2$,

$$\mathbf{D}(\mathbf{x}) = D_1 \mathbf{1}_{[\mathbf{x} \in \mathcal{A}_1]} + D_2 \mathbf{1}_{[\mathbf{x} \in \mathcal{A}_2]}.$$

[A2 :] The drift vector $\mathbf{v}$ is weakly incompressible in $\mathcal{A}_1$ and $\mathcal{A}_2$. i.e. $\nabla \cdot \mathbf{v} = 0$ in $\mathcal{A}_1$ and $\mathcal{A}_2$ and, $[\mathbf{v} \cdot \eta] = 0$ on $\mathcal{S}$, where in here and throughout this chapter η is the unit normal to the surface $\mathcal{S}$ and for any $\mathbf{x}_0 \in \mathcal{S}$, $[\mathbf{v} \cdot \eta(\mathbf{x}_0)] = \lim_{\substack{\mathbf{x} \to \mathbf{x}_0 \\ \mathbf{x} \in \mathcal{A}_1}} \mathbf{v}(\mathbf{x}) \cdot \eta(\mathbf{x}_0) - \lim_{\substack{\mathbf{x} \to \mathbf{x}_0 \\ \mathbf{x} \in \mathcal{A}_2}} \mathbf{v}(\mathbf{x}) \cdot \eta(\mathbf{x}_0)$.

[A3 :] At the interface $\mathcal{S}$, the function c satisfies

$$\lim_{\substack{\mathbf{x} \to \mathbf{x}_0 \\ \mathbf{x} \in \mathcal{A}_1}} \lambda \frac{\partial c(t, \mathbf{x})}{\partial \eta(\mathbf{x}_0)} = \lim_{\substack{\mathbf{x} \to \mathbf{x}_0 \\ \mathbf{x} \in \mathcal{A}_2}} (1 - \lambda) \frac{\partial c(t, \mathbf{x})}{\partial \eta(\mathbf{x}_0)} \tag{4.2}$$

$$\lim_{\substack{\mathbf{x} \to \mathbf{x}_0 \\ \mathbf{x} \in \mathcal{A}_1}} c(t, \mathbf{x}) = \lim_{\substack{\mathbf{x} \to \mathbf{x}_0 \\ \mathbf{x} \in \mathcal{A}_2}} c(t, \mathbf{x}) \tag{4.3}$$

for any $\mathbf{x}_0 \in \mathcal{S}$, where $0 \leq \lambda \leq 1$.

For $\bar{\lambda}(\mathbf{x}) = \lambda \mathbf{1}_{[\mathbf{x}\in\mathcal{A}_1]} + (1-\lambda)\mathbf{1}_{[\mathbf{x}\in\mathcal{A}_2]}$ the conditions (4.2) and (4.3) can be denoted in short by

$$\left[\bar{\lambda}\frac{\partial c}{\partial \eta}\right] = 0, \tag{4.4}$$

$$\text{and} \qquad [c] = 0. \tag{4.5}$$

[A4 :] The reaction rate R is bounded measurable function.

If we choose $\lambda = \dfrac{D_1}{D_1 + D_2}$, then the interface condition (4.4) becomes $\left[\mathbf{D}\dfrac{\partial c}{\partial \eta}\right] = 0$ on $\mathcal{S}$. Also since $\mathbf{v}$ is weakly incompressible on $\mathcal{A}_1 \cup \mathcal{A}_2$ and c is continuous everywhere, we get $\left[\mathbf{D}\dfrac{\partial c}{\partial \eta} - \mathbf{v}c\cdot\eta\right] = 0$ on $\mathcal{S}$, which is the continuity of flux across the interface.

Our objective in this chapter is to find the unique stochastic process associated with this convection reaction-diffusion equation (4.1) with the interface conditions (4.4) and (4.5). That being said, we state our first main theorem of this chapter as follows:

Theorem 4.1.1. *There exist a unique stochastic process* $\mathbf{X}$ *with* $\mathbf{X}_0 = \mathbf{x}$ *defined on a probability space* $(\Omega, \mathcal{F}, \mathbb{P})$ *such that the solution to the equation (4.1) with conditions [A1]-[A4] is given by* $c(t, \mathbf{x}) = \mathbb{E}_{\mathbf{x}} c_0(\mathbf{X}_t)$ *for all* $t \geq 0$ *and* $\mathbf{x} \in \mathbb{R}^n$. *i.e.* $\mathbf{X}$ *is the stochastic process associated with the differential equation (4.1) with the interface conditions (4.4) and (4.5).*

It is quite challenging to work with interfaces on a more general geometry than planar interfaces. The natural approach to tackle this general geometry of the interface is by flattening it out to a planar interface. We do so by using a special type of change of coordinate function that preserves the conditions at the interface. i.e. we choose a coordinate system $\mathbf{y} = (y_1, ..., y_n)$ in which the interface $\mathcal{S}$ is the hyperplane $y_n = 0$ and the normal derivative at $y_n = 0$ is equal to the normal derivative at the interface $\mathcal{S}$ in the original coordinate system. All the necessary conditions for this change of coordinate function is given later in the section 4.5. In that section we denote the change of coordinate function by Φ^{-1}. i.e. $\Phi(\mathbf{y}) = (\phi_1(\mathbf{y}), ..., \phi_n(\mathbf{y})) = \mathbf{x}$.

Denote $\widetilde{c}(t,\mathbf{y}) = c(t,\Phi(\mathbf{y}))$, $\widetilde{\mathbf{D}}(\mathbf{y}) = D_1\mathbb{I}_{[y_n\geq 0]} + D_2\mathbb{I}_{[y_n<0]}$, $\widetilde{\lambda}(\mathbf{y}) = \lambda\mathbb{I}_{[y_n\geq 0]} + (1-\lambda)\mathbb{I}_{[y_n<0]}$ and the matrices $\mathbf{a} = (a_{ij})_{n\times n}$, $\mathbf{b} = (b_j)_{n\times 1}$ are such that

$$a_{ij} = \sum_{k=1}^{n} \frac{\partial y_i}{\partial \phi_k}\frac{\partial y_j}{\partial \phi_k} \quad \text{and} \quad b_j = \sum_{k=1}^{n} \frac{\partial^2 y_j}{\partial \phi_k^2} \qquad \text{for } i,j \in \{1,2,...,n\}. \tag{4.6}$$

Then the equation (4.1) and the interface conditions (4.4), (4.5) in this new coordinate system can be written as follows.

$$\frac{\partial \tilde{c}}{\partial t} = \frac{1}{2}\widetilde{\mathbf{D}}(\mathbf{y})\sum_{i,j=1}^{n} a_{ij}(\mathbf{y})\frac{\partial^2 \tilde{c}(\mathbf{y})}{\partial y_i \partial y_j} + \sum_{j=1}^{n}\Big(\frac{1}{2}\widetilde{\mathbf{D}}(\mathbf{y})b_j(\mathbf{y}) - v_j(\mathbf{y})\Big)\frac{\partial \tilde{c}(\mathbf{y})}{\partial y_j} - (\nabla \mathbf{v}(\mathbf{y}) - R(\mathbf{y}))\tilde{c}(\mathbf{y}) \tag{4.7}$$

$$\Big[\widetilde{\lambda}(\mathbf{y})\frac{\partial \tilde{c}(t,\mathbf{y})}{\partial y_n}|_{(y_1,...y_{n-1},0)}\Big] = 0 = \big[\tilde{c}\big] \tag{4.8}$$

$$\tilde{c}(0,\mathbf{y}) = \tilde{c}_0(\mathbf{y}) \tag{4.9}$$

The complete description of the derivation of equation (4.7) and interface conditions (4.8), (4.9) is given in section 4.5. Now we are ready to state our second main theorem in this chapter as follows:

Theorem 4.1.2. *There exists a unique stochastic process associated with the PDE (4.7) and interface conditions (4.8), (4.9). i.e. there exists a unique stochastic process* $\mathbf{Y}$ *such that* $\widetilde{c}(t,\mathbf{y}) = \mathbb{E}_{\mathbf{y}}\widetilde{c}_0(\mathbf{Y}_t)$ *for all* $t \geq 0$ *and* $\mathbf{y} \in \mathbb{R}^n$.

Notice that the Theorem 4.1.1 is a consequence of this preceding theorem. Assuming the Theorem 4.1.2, the proof of Theorem 4.1.1 is immediate as it is only undoing the change of coordinates. We dedicated the section 4.6 for the proof of Theorem 4.1.2.

One important method of proving the existence and uniqueness of a stochastic process associated with a PDE is by formulating the Martingale problem associated to the PDE and proving the existence and uniqueness of solutions to it. Following is the basic definition of the Martingale problem. The complete definition is given in the section 4.2.

Given a differential operator $\mathcal{L}$ acting on functions in $\mathcal{A}(\mathcal{L})$, a process $\mathbf{X}_t^{\mathbf{x}}$ on some probability space $(\Omega, \mathcal{F}_t, \mathbb{P})$ adapted to the filtration $\mathcal{F}_t$ is said to be a solution to the Martingale problem associated to the operator $\mathcal{L}$ if for all $f \in \mathcal{A}(\mathcal{L})$

$$f(\mathbf{X}_t^{\mathbf{x}}) - \int_0^t \mathcal{L}f(\mathbf{X}_u^{\mathbf{x}})\mathrm{d}u \quad \text{is a } \ \mathcal{F}_t \ \text{ martingale}$$

and

$$\mathbb{P}(\mathbf{X}_0^{\mathbf{x}} = \mathbf{x}) = 1$$

If this stochastic process has a transition probability density function, say $p(t, x, y)$, satisfying regularity conditions and for any $A \in \mathcal{F}_t$, $\mathbb{P}(\mathbf{X}_t^{\mathbf{x}} \in A) = \int_A p(t, x, y)dy$. Then for any fixed y, $p(t, x, y)$ satisfies

$$\frac{\partial p}{\partial t} = \mathcal{L}p \quad \text{with} \quad p(0, x, y) = \delta_x(y) \tag{4.10}$$

Then we say this p is a fundamental solution of the PDE (4.10).

To formulate the Martingale problem for the problem in hand, one looks at the differential operator associated with the spatial variable of the PDE (4.7)

$$\mathcal{L}f = \frac{1}{2}\widetilde{\mathbf{D}}(\mathbf{y}) \sum_{i,j=1}^{n} a_{ij}(\mathbf{y}) \frac{\partial^2 f(\mathbf{y})}{\partial y_i \partial y_j} + \sum_{j=1}^{n} \Big(\frac{1}{2}\widetilde{\mathbf{D}}(\mathbf{y}) b_j(\mathbf{y}) - v_j(\mathbf{y}) \Big) \frac{\partial f(\mathbf{y})}{\partial y_j} - (\nabla \mathbf{v}(\mathbf{y}) - R(\mathbf{y})) f(\mathbf{y}) \tag{4.11}$$

The classical martingale problem is first introduced in Stroock and Varadhan (1979) for operators acting on C^2 functions. In Stroock and Varadhan (1979), it is established very useful results of formulating the martingale problem for operators having continuous coefficients. In Stroock (1987), it is extended some results of Stroock and Varadhan (1979) for more general coefficients. Later in Cerutti and Fabes (1991), uniqueness results of the martingale problem were extended for diffusion coefficients of finitely many discontinuities. Again in Bass and Pardoux (1987), it is extended the existence and uniqueness results for differential operators having piecewise constant diffusion coefficients on partition of $\mathbb{R}^n$ consists of finitely many polyhedral. In all these extensions the domain of the differential operator remains as real valued C^2 functions. But in our problem the differential operator (4.11) acts on functions in $\mathcal{D}_\lambda = \left\{ f \in C(\mathbb{R}^n) \cap C^2(\mathcal{A}_1 \cup \mathcal{A}_2) \mid \left[\widetilde{\lambda}\frac{\partial f}{\partial y_n}\right] = 0 \right\}$. Thus, results for martingale problem alone are not sufficient to find the associated stochastic process to our problem.

Our first step in proving the Theorem 4.1.2 is to find the stochastic differential equation (SDE) associated with the PDE and the interface conditions (4.7). Throughout this chapter, when we say "SDE associated with a PDE (or a differential operator)", we mean that the solution to this SDE is the stochastic process associated with the PDE (or differential operator). Since the function $\widetilde{c}$ in (4.7) is not C^2 in spatial variables, Itô formula does not apply in here. Even the more general Itô-Tanaka formula does not apply here as the local time term in the Itô-Tanaka formula is only defined in one dimension. We use the Peskir's change of variable formula with local time on a surface for this. More details on Peskir's change of variable formula is given in section 4.4.

In general, the interface condition in the PDE is captured by a local time term in its associated stochastic differential equation. In Le Gall (1982), the existence and uniqueness of solutions to one dimensional stochastic differential equations with local time term is established. But no such general result exists for higher dimensional stochastic differential equations with local time term. We prove the existence and the uniqueness of the solution to our SDE with the local time term by establishing a unique relationship between the solutions to this SDE with another stochastic process (in Section 4.6 we denote it by $\widehat{\mathbf{Z}}$) whose stochastic differential equation does not have a local time term. Then we use the formulation of Martingale problem to prove the existence and uniqueness of the process $\widehat{\mathbf{Z}}$.

The organization of this chapter is as follows. In the next section we introduce the Martingale problem and state some important theorems and lemmas that are going to use later. In Section 4.3, we introduce the random time change and use it to show that the local time of skew Brownian motion is discontinuous at zero. In Section 4.4, we state the Peskir's change of variable formula. In Section 4.5, we give the complete description of derivation of equation (4.7) and interface conditions (4.8), (4.9). In Section 4.6, we prove the Theorem 4.1.2. In Section 4.7, we do an example of finding the stochastic process associated with the diffusion equation in radially symmetric domain with an interface on a sphere. Finally in Section 4.8, we introduce the problem of finding a stochastic process associated with a PDE with more general geometry of the interface as finding solutions to corresponding Skorohod problem.

4.2 Martingale Problem

As mentioned in the introduction, a few different approaches are available to construct diffusion processes associated with linear second order parabolic PDEs. These diffusion processes are Markov processes and thus their transition probabilities will illustrate the process completely.

Beginning with the seminal work of Stroock and Varadhan (1969), martingale problems have proved to be an important tool in the construction and analysis of Markov processes complementing the theory of semi-groups and their generators. Martingale problems were used to construct and study properties of multidimensional diffusions (Stroock and Varadhan (1979)), Infinite particle systems and Icing models (Holley and Stroock (1976)), processes associated with Boltzman equation (Tanaka (1978)).

The basic idea here is to show that a certain expression involving the diffusion process and its generator makes a martingale.

Let us consider an operator of the form

$$\mathcal{L} = \sum_{i,j=1}^{n} a_{ij}(\mathbf{x}) \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i(\mathbf{x}) \frac{\partial}{\partial x_i}. \tag{4.12}$$

where the coefficients a_{ij}, b_i are locally bounded Borel measurable functions on $\mathbb{R}^n$.

Following we define the martingale problem associated with the operator (4.12) as defined in Oksendal (2003).

Definition 4.2.1. *(Martingale Problem). We say that a probability measure $P^{\mathbf{x}}$ on $(C([0,\infty);\mathbb{R}^n),\mathcal{B})$ such that $P^{\mathbf{x}}(\omega_o = \mathbf{x}) = 1$ solves the martingale problem for $\mathcal{L}$ (or $\mathbf{a} = ((a_{ij}))$ and $\mathbf{b} = ((b_i))$) defined in (4.12), if the process*

$$M_t := f(\omega_t) - \int_0^t \mathcal{L}f(\omega_s)ds, \quad M_0 = f(\mathbf{x}) \quad a.s. \;\; P^{\mathbf{x}}$$

is a $P^{\mathbf{x}}$ martingale with respect to $\mathcal{B}_t$, for all $f \in C_0^2(\mathbb{R}^n)$. The martingale problem is called well posed if there is a unique measure $P^{\mathbf{x}}$ for each starting point $\mathbf{x}$ solving the martingale problem.

The main idea used in martingale problem is the Itô formula. To see this let us look at an example. Let

$$d\mathbf{X}_t^x = \sigma(\mathbf{X}_t^x)d\mathbf{B}_t + \mathbf{b}(\mathbf{X}_t^x)dt \tag{4.13}$$

be an Itô diffusion in $\mathbb{R}^n$ with generator $\mathcal{A}$. This generator $\mathcal{A}$ is given by

$$\mathcal{A} = \frac{1}{2}\sum_{i,j=1}^n a_{ij}(\mathbf{x})\frac{\partial^2}{\partial x^{(i)}\partial x^{(j)}} + \sum_{j=1}^n b_j(\mathbf{x})\frac{\partial}{\partial x^{(j)}} \tag{4.14}$$

where $\mathbf{a} = ((a_{ij})) = \sigma\sigma^T$ and $\mathbf{b} = ((b_j))$.

Now for $f \in C_0^2(\mathbb{R}^n)$, by Itô formula one has

$$f(\mathbf{X}_t^x) = f(\mathbf{x}) + \int_0^t \mathcal{A}f(\mathbf{X}_s^x)ds + \int_0^t \nabla f^T(\mathbf{X}_s^x)\sigma(\mathbf{X}_s^x)d\mathbf{B}_s.$$

Define

$$M_t = f(\mathbf{X}_t^x) - \int_0^t \mathcal{A}f(\mathbf{X}_s^x)ds. \tag{4.15}$$

Then since Itô integrals are martingales we have that M_t is a martingale with respect to the filtration $\{\mathcal{M}_t\}$.

If we identify each $\omega \in \Omega$ in the probability space $(\Omega, \mathcal{M}, Q^{\mathbf{x}})$ with the function

$$\omega_t = \omega(t) = \mathbf{X}_t^x(\omega),$$

then this identifies the probability space $(\Omega, \mathcal{M}, Q^{\mathbf{x}})$ with $(C([0,\infty);\mathbb{R}^n), \mathcal{B}, \widetilde{Q}^{\mathbf{x}})$. This implies that the law of $\mathbf{X}_t^x$ on Borel σ-algebra $\mathcal{B}$ of $C([0,\infty);\mathbb{R}^n)$ is $\widetilde{Q}^x$. Then one has that the process defined in (4.15) is a $\widetilde{Q}^x$ - martingale with respect to the Borel σ-algebra $\mathcal{B}$ on $C([0,\infty);\mathbb{R}^n)$.

This says that $\widetilde{Q}^x$ solves the martingale problem associated with the operator $\mathcal{A}$ defined in (4.14) whenever $\mathbf{X}^x$ is a weak solution to the stochastic differential equation (4.13). Conversely it can be shown that if $\widetilde{P}^x$ solves the martingale problem for the operator $\mathcal{A}$ in (4.14) starting at x, for all $x \in \mathbb{R}^n$, then there exists a weak solution $\mathbf{X}^x$ of the stochastic differential equation (4.13).

We rephrase the Theorem 2.6 in page 91 of Stroock (1987) in the following Lemma that shows having a solution to the martingale problem leads to an existence of a weak solution to the stochastic differential equation (4.13).

Lemma 4.2.2. *Let* $\mathbf{a}$ *be a symmetric and positive definite matrix with each entries bounded measurable functions, and* $\mathbf{b}$ *be a bounded measurable function. Suppose that* P^x *solves the martingale problem for* $\mathbf{a}$ *and* $\mathbf{b}$ *for any starting point* $x \in \mathbb{R}^n$. *Given a measurable* $\sigma : \mathbb{R}^n \to Hom(\mathbb{R}^n;\mathbb{R}^n)$ *satisfying* $\mathbf{a} = \sigma\sigma^T$, *there is a n-dimensional Brownian motion* $(\mathbf{B}_t, \mathcal{F}_t, Q)$ *on some probability space* $(\Omega, \mathcal{F}, Q)$ *and a continuous* $\{\mathcal{F}_t\}$*-progressively measurable function* $\mathbf{X} : [0,\infty) \times \Omega \to \mathbb{R}^n$ *such that*

$$\begin{cases} d\mathbf{X}_t = \sigma(\mathbf{X}_t)d\mathbf{B}_t + \mathbf{b}(\mathbf{X}_t)dt \\ \mathbf{X}_0 = x \end{cases}$$

for $t \geq 0$ *(a.s. Q) and* $P^x = Q \circ \mathbf{X}(\cdot)^{-1}$.

This weak solution is a Markov process if and only if the martingale problem corresponding to the differential operator $\mathcal{A}$ defined in (4.14) is well posed, see for example Stroock and Varadhan (1979). It is important for the stochastic process to be a Markov process as it makes the process to have transition probabilities. Thus for applications point of view, well posedness of a martingale problem is crucial.

When the coefficients $\mathbf{a}$ and $\mathbf{b}$ are Lipschitz, the martingale problem for $\mathbf{a}$ and $\mathbf{b}$ is well posed; see for example Stroock and Varadhan (1979). Question is that how far one can relax the conditions on $\mathbf{a}$ and $\mathbf{b}$ to have well posedness for the martingale problem.

Uniqueness of solutions to martingale problem is a local property. That is, for the global uniqueness of the solution to a martingale problem, one only needs to check the locally uniqueness of the solution. To understand this localization of the uniqueness, first we give the definition of locally well posedness of a martingale problem as given in Stroock (1987). To set some notations, define $S(\mathbb{R}^n)$ be the set of symmetric and positive definite $n \times n$ matrices.

Definition 4.2.3. *Given a bounded measurable* $\mathbf{a} : \mathbb{R}^n \to S(\mathbb{R}^n)$ *and* $\mathbf{b} : \mathbb{R}^n \to \mathbb{R}^n$*, we say that the martingale problem for* $\mathbf{a}$ *and* $\mathbf{b}$ *is locally well posed if* $\mathbb{R}^n$ *can be covered by open sets* U *with the property that there exist bounded measurable* $\mathbf{a}_U : \mathbb{R}^n \to S(\mathbb{R}^n)$ *and* $\mathbf{b}_U : \mathbb{R}^n \to \mathbb{R}^n$ *such that* $\mathbf{a}|_U = \mathbf{a}_U|_U$ *and* $\mathbf{b}|_U = \mathbf{b}_U|_U$*, and the martingale problem associated with* $\mathbf{a}_U$ *and* $\mathbf{b}_U$ *is well posed.*

The following lemma shows that one only needs local well posedness of the martingale problem for the global well posedness.

Lemma 4.2.4. *Let* $\mathbf{a} : \mathbb{R}^n \to S(\mathbb{R}^n)$ *and* $\mathbf{b} : \mathbb{R}^n \to \mathbb{R}^n$ *be bounded measurable functions and define the differential operator associated with the martingale problem for* $\mathbf{a}$ *and* $\mathbf{b}$ *accordingly. If the martingale problem for* $\mathbf{a}$ *and* $\mathbf{b}$ *is locally well posed, then it is in fact well posed.*

Proof. See Theorem 3.5 in Stroock (1987). □

Another important property of the martingale problem is that under certain conditions on $\mathbf{a}$ and $\mathbf{b}$, there is a one-to-one correspondence between well posedness of the martingale problem for $\mathbf{a}$ and $\mathbf{0}$, and well posedness of the martingale problem for $\mathbf{a}$ and $\mathbf{b}$. The important technique used in here is well known Cameron-Martin-Girsanov theorem.

More precisely, suppose **a** be symmetric and uniformly positive definite i.e. there is $\lambda > 0$ such that

$$\langle \theta, \mathbf{a}(x)\theta \rangle \geq \lambda \|\theta|^2 \quad x \in \mathbb{R}^n \text{ and } \theta \in \mathbb{R}^n. \tag{4.16}$$

Also suppose that the martingale problem for **a** and **0** is well posed for any starting point $x \in \mathbb{R}^n$. Let us denote P^x as the probability measure that solves the martingale problem for **a** and **0**. We already mentioned that having a unique solution to the martingale problem for **a** and **0** implies that the stochastic differential equation

$$d\mathbf{X}_t = \sigma(\mathbf{X}_t)d\mathbf{B}_t$$

where $\mathbf{a} = \sigma\sigma^T$, has a unique solution, say $\mathbf{X}^{\mathbf{a}}$.

Now let **b** be a bounded measurable function and define the probability measure Q^x through the following Radon-Nikodym derivative;

$$\frac{dQ^x}{dP^x}|_{\mathcal{M}_t} = \exp\left[\int_0^t \langle \mathbf{a}^{-1}\mathbf{b}(\mathbf{X^a}_s), d\mathbf{X^a}_s\rangle - \frac{1}{2}\int_0^t \langle \mathbf{b}, \mathbf{a}^{-1}\mathbf{b}\rangle(\mathbf{X^a}_s)ds\right], \quad \text{for all } t \geq 0 \tag{4.17}$$

Then this Q^x is the unique solution to the martingale problem for **a** and **b**. For more details see Theorem 6.4.3 in Stroock and Varadhan (1979).

The following lemma gives well-posedness of a martingale problem for more general diffusion coefficient **a**.

Theorem 4.2.5. *Let* **a** *be an uniformly positive definite continuous matrix on* $\mathbb{R}^n$ *except possibly on a countable set with at most one cluster point. Then the martingale problem for* **a** *is well-posed.*

Proof. See Theorem 4 in Cerutti and Fabes (1991). □

Even in this most general result (Theorem 4.2.5), it is required that the matrix **a** to be continuous everywhere except at most on countable set. But in applications one would often encounter problems involving diffusion coefficient matrices **a** which are discontinuous on surfaces. If the discontinuity of **a** can be removed by multiplying it by a strictly positive real valued function, the well posedness of the martingale problem can still be achieved through a technique called random time change. In the following section we describe the random time change. As an application of it we give an independent proof to show that the local time of skew Brownian motion has a spatial discontinuity at zero.

4.3 Random time change in $\mathbb{R}^n$

It is possible to transform one stochastic process into another by stretching and shrinking the time-scale, sometimes in a deterministic manner, more often by means of a random change of time-scale which depends on the realized trajectory of the process you started with. One example is the transformation of point processes to Poisson processes. There are results that use this random time change in the context of martingale problem.

This random time change involves stopping times. If P is a solution to the martingale problem associated with some operator $\mathcal{L}$ on $\Omega = C([0,\infty),\mathcal{O})$, then there exists a stochastic process X in the probability space$(\Omega,\mathcal{F}_t,\mathbb{P})$ whose law is P such that

$$f(X(t))) - f(X(0)) - \int_0^t (\mathcal{L}f)(X(s))\ ds$$

is a P-martingale. We now consider the stopping times $\{\tau_t\}$, defined by,

$$\int_0^{\tau_t(\omega)} \varphi(X(s,\omega))ds = t \tag{4.18}$$

where φ is a uniformly positive measurable function on $\mathcal{O}$. Now define a map $S_\varphi : \Omega \to \Omega$ by

$$X(t, S_\varphi^{-1}(\omega)) = X(\tau_t(\omega),\omega), \quad t \geq 0, \quad \omega \in \Omega$$

which is called the random time change of the process X. If we define the new process $\tilde{X}(\tau,\omega) := X(t,\omega)$, then the new process $\tilde{X}(\tau,\omega)$ is associated with the operator $\varphi\mathcal{L}$ and $P \circ S_\varphi^{-1}$ solves the martingale problem for $\varphi\mathcal{L}$.

For more information on random time change see Theorem 6.5.2 in Stroock and Varadhan (1979).

For an example, consider $L = \frac{1}{2}\frac{\partial^2}{\partial x^2}$. Then we have the PDE

$$\frac{\partial}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial x^2}. \tag{4.19}$$

It is well known that the standard Brownian motion B is the associated stochastic process for (4.19). Let us take $\varphi = D$ a constant. Then we have that $D\tau = t$. So in new time scale, (4.19) becomes

$$\frac{\partial}{\partial \tau} = \frac{D}{2}\frac{\partial^2}{\partial x^2}. \tag{4.20}$$

Now if we assume X be the stochastic process associated with this PDE (4.20), then we have $X(\tau,\omega) = B(t,\omega) = B(D\tau,\omega)$. From the scaling property of Brownian motion we have that $X(\tau,\omega) = \sqrt{D}B(\tau,\omega)$, which is what one would expect.

As an application of this random time change, we will show that the local time process of skew Brownian motion is discontinuous at zero.

4.3.1 Spatial discontinuity of the local time of skew Brownian motion at zero

It is well known that skew Brownian motion with parameter α, $B^{(\alpha)}$, satisfies the following PDE and the interface condition:

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2} \tag{4.21}$$

$$\alpha\frac{\partial u}{\partial x}|_{x=0^+} = (1-\alpha)\frac{\partial u}{\partial x}|_{x=0^-}. \tag{4.22}$$

Now we change the spatial variable and define $v(t,x) = u(t, 2\alpha(x)x)$ where

$$\alpha(x) = \begin{cases} \alpha & \text{if } x > 0 \\ 1-\alpha & \text{if } x < 0. \end{cases}$$

Then this new function v satisfies the following PDE:

$$\frac{\partial v}{\partial t} = \frac{1}{2}\frac{1}{4\alpha^2(x)}\frac{\partial^2 v}{\partial x^2} \tag{4.23}$$

$$\frac{\partial u}{\partial x}|_{x=0^+} = \frac{\partial u}{\partial x}|_{x=0^-}. \tag{4.24}$$

From the change of spatial variable we have that $X = \frac{1}{2\alpha(B^{(\alpha)})}B^{(\alpha)}$ is the stochastic process associated with (4.23). Now chose a new time scale λ satisfying $\frac{dt}{d\lambda} = 4\alpha^2(X(t))$. Then in new time scale we have

$$\frac{\partial v}{\partial \lambda} = \frac{1}{2}\frac{\partial^2 v}{\partial x^2} \tag{4.25}$$

for which B is the associated stochastic process. Then we have that $B(t,\omega) = X(\lambda^{-1}(t),\omega)$ $= \frac{1}{2\alpha(B^{(\alpha)}(\lambda^{-1}(t),\omega))}B^{(\alpha)}(\lambda^{-1}(t),\omega)$.

Now look at the one sided local time of skew Brownian motion at zero as follows:

$$\begin{aligned} L^{0+}_{\lambda^{-1}(t)}(B^{(\alpha)}) &= \lim_{\epsilon\downarrow 0}\frac{1}{\epsilon}\int_0^{\lambda^{-1}(t)} \mathbb{I}_{[0\leq B^{(\alpha)}(s)<\epsilon]}\ d\langle B^{(\alpha)}, B^{(\alpha)}\rangle_s \\ &= \lim_{\epsilon\downarrow 0}\frac{1}{\epsilon}\int_0^{\lambda^{-1}(t)} \mathbb{I}_{[0\leq 2\alpha X(s)<\epsilon]}\ ds \\ &= \lim_{\epsilon\downarrow 0}\frac{1}{\epsilon}\int_0^{\lambda^{-1}(t)} \mathbb{I}_{[0\leq B(\lambda(s))<\frac{\epsilon}{2\alpha}]}\ ds \end{aligned}$$

By change of variable $\lambda(s) = u$ and relabeling some terms we get;

$$\begin{aligned} L^{0+}_{\lambda^{-1}(t)}(B^{(\alpha)}) &= \frac{4\alpha^2}{2\alpha}\lim_{\frac{\epsilon}{2\alpha}\downarrow 0}\frac{2\alpha}{\epsilon}\int_0^t \mathbb{I}_{[0\leq B(u)<\frac{\epsilon}{2\alpha}]}\ du \\ &= 2\alpha L^{0+}_t(B) \end{aligned}$$

Similar computation yields,

$$L^{0^-}_{\lambda^{-1}(t)}(B^{(\alpha)}) = L^{0^-}_t(B).$$

These two equalities valid for any $t \geq 0$. Since the local time of Brownian motion is continuous in space, we have

$$2(1-\alpha)L^{0^+}_t(B^{(\alpha)}) = 2\alpha L^{0^-}_t(B^{(\alpha)}),$$

which shows that the local time is discontinuous at zero.

4.4 Peskir's change of variable formula

To connect a standard diffusion process to a PDE, we often use Itô formula. But for more general diffusion processes whose stochastic differential equation has a local time term, this well known Itô formula is not sufficient. For example, one dimensional skew Brownian motion, which is a version of a Brownian motion but twisted at the origin. In this case one needs to use more generalized version of Itô formula called Itô-Tanaka formula. But in higher dimensions, this formula can be used only when the diffusion matrix is diagonal and the local time is on a hyperplane. But to capture the local time of a process on more general surface in higher dimension, one needs to have a more sophisticated formula. Peskir's change of variable formula with local time on surfaces is the generalized version of the Itô-Tanaka formula which can be used in the latter case.

In the following theorem we state the Peskir's change of variable formula given in Peskir (2006). We rephrase it so as to make the notations compatible with rest of the chapter. For convenience we have the following notation for a function h;

$$h(\bar{x}_1, ..., \bar{x}_{n-1}, \bar{x}_n^+) = \lim_{\substack{\mathbf{x} \to \bar{\mathbf{x}} \\ g(x_1,...,x_{n-1}) < x_n}} h(\mathbf{x})$$

Theorem 4.4.1. *Let* $\mathbf{X} = (X^1, ..., X^n)$ *be a continuous semimartingale and let* $g : \mathbb{R}^{n-1} \to \mathbb{R}$ *be a continuous function such that the process* $g^{\mathbf{X}} = g(X^1, ..., X^{n-1})$ *is a semimartingale. Set* $\mathcal{A}_1 = \{(x_1, x_2, ..., x_n) \in \mathbb{R}^n | x_n > g(x_1, x_2, ..., x_{n-1})\}$ *and* $\mathcal{A}_2 = \{(x_1, x_2, ..., x_n) \in \mathbb{R}^n | x_n < g(x_1, x_2, ..., x_{n-1})\}$*. Suppose that a continuous function* $F : \mathbb{R}^n \to \mathbb{R}$ *is given such that* F *is* $C^{i_1,...,i_n}$ *on* $\bar{\mathcal{A}}_1$ *and* $\bar{\mathcal{A}}_2$ *where each* i_k *equals 1 or 2 depending on whether* X^k *is of bounded variation or not. Then the following change of variable formula holds:*

$$F(\mathbf{X}_t) = F(\mathbf{X}_0) + \sum_{i=1}^{n} \int_0^t \frac{\partial F}{\partial x_i}(X_s^1, ..., X_s^{n-1}, X_s^n \mp)\ dX_s^i$$
$$+ \frac{1}{2} \sum_{i,j=1}^{n} \int_0^t \frac{\partial^2 F}{\partial x_i \partial x_j}(X_s^1, ..., X_s^{n-1}, X_s^n \mp)\ d\langle X^i, X^j \rangle_s$$
$$+ \frac{1}{2} \int_0^t \left(\frac{\partial F}{\partial x_n}(X_s^1, ..., X_s^{n-1}, X_s^n +) - \frac{\partial F}{\partial x_n}(X_s^1, ..., X_s^{n-1}, X_s^n -) \right) \mathbb{I}_{(X_s^n = g_s^{\mathbf{X}})}\ dL_s^{g\pm}(\mathbf{X})$$

where one sided local times of $\mathbf{X}$ *on the surface* b *are given by:*

$$L_s^{g+}(\mathbf{X}) = \mathbb{P} - lim_{\epsilon \downarrow 0} \frac{1}{\epsilon} \int_0^s \mathbb{I}_{[0 \le X_r^n - g_r^{\mathbf{X}} < \epsilon]}\ d\langle X^n - g^{\mathbf{X}}, X^n - g^{\mathbf{X}} \rangle_r$$

and

$$L_s^{g-}(\mathbf{X}) = \mathbb{P} - lim_{\epsilon \downarrow 0} \frac{1}{\epsilon} \int_0^s \mathbb{I}_{[-\epsilon < X_r^n - g_r^{\mathbf{X}} \le 0]}\ d\langle X^n - g^{\mathbf{X}}, X^n - g^{\mathbf{X}} \rangle_r.$$

4.5 Flattening the Interface

Recall that in the introduction, we assume g is a C^2 real valued function in $\mathbb{R}^{n-1}$. Denote the graph of g by $\mathcal{S} = \{(x_1, x_2, ..., x_n) \in \mathbb{R}^n | x_n = g(x_1, x_2, ..., x_{n-1})\}$. Denote the two regions separated by $\mathcal{S}$ by $\mathcal{A}_1 = \{(x_1, x_2, ..., x_n) \in \mathbb{R}^n | x_n > g(x_1, x_2, ..., x_{n-1})\}$ and $\mathcal{A}_2 = \{(x_1, x_2, ..., x_n) \in \mathbb{R}^n | x_n < g(x_1, x_2, ..., x_{n-1})\}$. Then for a real valued function $c \in C([0, \infty), \mathbb{R}^n) \cap C^{1,2}([0, \infty), \mathcal{A}_1 \cup \mathcal{A}_2)$, we consider

$$\frac{\partial c}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{v}c) = \frac{1}{2} \nabla_{\mathbf{x}} \cdot (\mathbf{D}(\mathbf{x}) \nabla_{\mathbf{x}} c) + R(\mathbf{x})c \quad t \ge 0, \quad \mathbf{x} \in \mathbb{R}^n \setminus \mathcal{S} \tag{4.26}$$

with the initial condition $c(0, \mathbf{x}) = c_0(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^n$ and the interface condition

$$\left[\bar{\lambda} \frac{\partial c}{\partial \eta} \right] = 0 = [c] \quad \text{on} \quad \mathcal{S}. \tag{4.27}$$

where $\bar{\lambda}(\mathbf{x}) = \lambda \mathbf{1}_{[\mathbf{x} \in \mathcal{A}_1]} + (1 - \lambda) \mathbf{1}_{[\mathbf{x} \in \mathcal{A}_2]}$ with $0 \le \lambda \le 1$ and η is the normal to the surface $\mathcal{S}$ and $\mathbf{D}(\mathbf{x}) = D_1 \mathbb{I}_{\mathcal{A}_1}(\mathbf{x}) + D_2 \mathbb{I}_{\mathcal{A}_2}(\mathbf{x})$ and R is a function in $\mathbb{R}^n$ and $\mathbf{v}$ is weakly incompressible in $\mathcal{A}_1$ and $\mathcal{A}_2$.

For $\mathbf{x} = (x_1, x_2, ..., x_n), \mathbf{y} = (y_1, y_2, ..., y_n) \in \mathbb{R}^n$, let us denote $\mathbf{x}' = (x_1, x_2, ..., x_{n-1})$ and $\mathbf{y}' = (y_1, y_2, ..., y_{n-1})$. Let's consider a change of coordinates Φ^{-1} satisfying following conditions:

i. $\Phi(\mathbf{y}) = (\phi_1(\mathbf{y}), \phi_2(\mathbf{y}), ..., \phi_n(\mathbf{y})) = \mathbf{x}$

ii. $\Phi(\mathbf{y}', 0)$

$= (\phi_1(\mathbf{y}', 0), \phi_2(\mathbf{y}', 0), ..., \phi_{n-1}(\mathbf{y}', 0), g(\phi_1(\mathbf{y}', 0), \phi_2(\mathbf{y}', 0), ..., \phi_{n-1}(\mathbf{y}', 0)))$

$= (\mathbf{y}', g(\mathbf{y}')) = (\mathbf{x}', g(\mathbf{x}'))$

iii. $\phi_n(\mathbf{y}) > g(\phi_1(\mathbf{y}), \phi_2(\mathbf{y}), ..., \phi_{n-1}(\mathbf{y}))$ if $y_n > 0$

iv. $\phi_n(\mathbf{y}) > g(\phi_1(\mathbf{y}), \phi_2(\mathbf{y}), ..., \phi_{n-1}(\mathbf{y}))$ if $y_n < 0$

v. for each $j \in \{1, 2, ..., n-1\}$, $\left.\dfrac{\partial \phi_j}{\partial y_n}\right|_{(\mathbf{y}',0)} = -\left.\dfrac{\partial g}{\partial x_j}\right|_{(\mathbf{y}',0)}$ and $\left.\dfrac{\partial \phi_n}{\partial y_n}\right|_{(\mathbf{y}^{n-1},0)} = 1$

Let us denote $\tilde{c}(t, \mathbf{y}) = c(t, \Phi(\mathbf{y})) = c(t, \mathbf{x})$, $\widetilde{\mathbf{D}}(\mathbf{y}) = \mathbf{D}(\Phi(\mathbf{y}))$ and $\widetilde{\lambda}(\mathbf{y}) = \bar{\lambda}(\Phi(\mathbf{y}))$. Then,

$$\widetilde{\mathbf{D}}(\mathbf{y}) = \begin{cases} D_1 & \text{if } \ y_n \geq 0 \\ D_2 & \text{if } \ y_n < 0 \end{cases}$$

and

$$\widetilde{\lambda}(\mathbf{y}) = \begin{cases} \lambda & \text{if } \ y_n \geq 0 \\ 1-\lambda & \text{if } \ y_n < 0 \end{cases}$$

Also from the properties *ii* and *v* we have,

$$\begin{aligned}
\frac{\partial \tilde{c}}{\partial y_n}\Big|_{(\mathbf{y}',0^\pm)} &= \Big[\sum_{i=1}^{n-1}\Big(\frac{\partial c}{\partial x_i}\frac{\partial x_i}{\partial y_n}\Big) + \frac{\partial c}{\partial x_n}\frac{\partial x_n}{\partial y_n}\Big]\Big|_{(\mathbf{y}',0^\pm)} \\
&= \Big[\sum_{i=1}^{n-1}\Big(\frac{\partial c}{\partial x_i}\frac{\partial \phi_i}{\partial y_n}\Big) + \frac{\partial c}{\partial x_n}\frac{\partial \phi_n}{\partial y_n}\Big]\Big|_{(\mathbf{y}',0^\pm)} \\
&= \Big[\sum_{i=1}^{n-1}\Big(\frac{\partial c}{\partial x_i}\Big|_{(\mathbf{y}',0^\pm)}\frac{\partial \phi_i}{\partial y_n}\Big|_{(\mathbf{y}',0^\pm)}\Big) + \frac{\partial c}{\partial x_n}\Big|_{(\mathbf{y}',0^\pm)}\frac{\partial \phi_n}{\partial y_n}\Big|_{(\mathbf{y}',0^\pm)}\Big] \\
&= \Big[-\sum_{i=1}^{n-1}\Big(\frac{\partial g}{\partial x_i}\frac{\partial c}{\partial x_i}\Big) + \frac{\partial c}{\partial x_n}\Big]\Big|_{(\mathbf{x}',g(\mathbf{x}'))^\pm}
\end{aligned}$$

Therefore we have that $\tilde{c} \in C([0,\infty),\mathbb{R}^n) \cap C^{1,2}([0,\infty),\mathbb{R}^n \setminus \{(\mathbf{y}',0)\})$ and the PDE (4.26) and the transmission condition (4.27) in new coordinate system

$$\frac{\partial \tilde{c}}{\partial t} = \frac{1}{2}\widetilde{\mathbf{D}}(\mathbf{y})\sum_{i,j=1}^{n} a_{ij}(\mathbf{y})\frac{\partial^2 \tilde{c}(\mathbf{y})}{\partial y_i \partial y_j} + \sum_{j=1}^{n}\Big(\frac{1}{2}\widetilde{\mathbf{D}}(\mathbf{y})b_j(\mathbf{y}) - v_j(\mathbf{y})\Big)\frac{\partial \tilde{c}(\mathbf{y})}{\partial y_j} - (\nabla\mathbf{v}(\mathbf{y}) - R(\mathbf{y}))\tilde{c}(\mathbf{y}) \tag{4.28}$$

$$\Big[\widetilde{\lambda}(\mathbf{y})\frac{\partial \tilde{c}(t,\mathbf{y})}{\partial y_n}|_{(\mathbf{y}',0)}\Big] = 0 = [\tilde{c}]$$

$$\tilde{c}(0,\mathbf{y}) = \tilde{c}_0(\mathbf{y})$$

where the matrices $\mathbf{a} = (a_{ij})_{n\times n}$ and $\mathbf{b} = (b_j)_{n\times 1}$ are as follows:

$$a_{ij} = \sum_{k=1}^{n}\frac{\partial y_i}{\partial \phi_k}\frac{\partial y_j}{\partial \phi_k} \quad \text{and} \quad b_j = \sum_{k=1}^{n}\frac{\partial^2 y_j}{\partial \phi_k^2} \qquad \text{for } i,j \in \{1,2,...,n\}. \tag{4.29}$$

Let us denote $\mathbf{k} = (k_j)_{n\times 1}$ where

$$k_j(\cdot) = \frac{1}{2}\widetilde{\mathbf{D}}(\cdot)b_j(\cdot) - v_j(\cdot) \qquad \text{for} \quad j = 1,2,...,n \tag{4.30}$$

and,

$$r(\cdot) = \nabla\mathbf{v}(\cdot) - R(\cdot) \tag{4.31}$$

Let us define the differential operator $\mathcal{L}^{\mathbf{Y}}$ acting on functions in the domain $\mathcal{D}_\lambda =$

$\Big\{f \in C(\mathbb{R}^n) \cap C^2(\mathbb{R}^n \setminus \{(\mathbf{y}', 0)\}) : \Big[\widetilde{\lambda}(\mathbf{y})\frac{\partial f(\mathbf{y})}{\partial y_n}|_{(\mathbf{y}',0)}\Big] = 0\Big\}$ as follows:

$$\mathcal{L}_{\mathbf{y}} = \frac{1}{2}\widetilde{\mathbf{D}}(\cdot)\sum_{i,j=1}^{n} a_{ij}(\cdot)\frac{\partial^2}{\partial y_i \partial y_j} + \sum_{j=1}^{n} k_j(\cdot)\frac{\partial}{\partial y_j} - r(\cdot) \tag{4.32}$$

Recall that our first main theorem (Theorem 4.1.2) is about the existence and uniqueness of the stochastic process associated with the PDE and interface conditions (4.28). Notice that proving this theorem is the same as proving the existence and uniqueness of the solution to the Martingale problem associated with the operator (4.32). The next section is dedicated for the proof of existence and uniqueness of the solution to the Martingale problem associated with the operator (4.32).

4.6 Existence and Uniqueness of the stochastic process for $\mathcal{L}_{\mathbf{y}}$

Notice that it is enough to prove the existence and uniqueness of the stochastic process associated with the operator $\mathcal{L}_{\mathbf{y}}$ with $r = 0$. From the Feynman-Kac formula, killing this process by an exponential random variable with rate $r(\cdot)$ gives the process $\mathbf{Y}$.

Let us define the differential operator $\widehat{\mathcal{L}}$ acting on functions in $\mathcal{D}_\lambda$ as follows:

$$\widehat{\mathcal{L}} = \frac{1}{2}\widetilde{\mathbf{D}}(\cdot)\sum_{i,j=1}^{n} a_{ij}(\cdot)\frac{\partial^2}{\partial y_i \partial y_j} + \sum_{j=1}^{n} k_j(\cdot)\frac{\partial}{\partial y_j}. \tag{4.33}$$

Now our primary task is to prove existence and uniqueness of the stochastic process associated with this operator $\widehat{\mathcal{L}}$.

The operator $\widehat{\mathcal{L}}$ defined in (4.33) is not acting on C^2 functions. The type of interface condition present in the domain of $\widehat{\mathcal{L}}$ translate to a local time term in the stochastic differential equation of its associated stochastic process. As we mentioned in the introduction, we first identify the stochastic differential equation associated with the operator (4.33) using the Peskir's change of variable formula. Then we show that this stochastic differential equation has a unique solution.

Let us consider the following stochastic differential equation.

$$d\mathbf{Z}_t = M(\mathbf{Z}_t)\ \sigma(\mathbf{Z}_t)d\mathbf{B}_t + \mathbf{k}(\mathbf{Z}_t)dt + \begin{pmatrix} 0 \\ . \\ . \\ . \\ 0 \\ \beta\ dL_t^{0^+}(\mathbf{Z}) \end{pmatrix} \tag{4.34}$$

where

$$L_t^{0^+}(\mathbf{Z}) = \lim_{\epsilon\downarrow 0}\frac{1}{\epsilon}\int_0^t \mathbf{1}_{[0\le Z_s^n<\epsilon]}d\langle Z^n, Z^n\rangle_s$$

is the one sided local time of Z^n at zero.

We state our main theorem in this section as follows.

Theorem 4.6.1. *The stochastic differential equation (4.34) has a unique solution for M piecewise constants on $y_n \geq 0$ and $y_n < 0$, β a constant, σ is a matrix such that $\sigma\sigma^T$ is uniformly positive definite whose entries are bounded continuous functions and $\mathbf{k}$ a vector whose entries are bounded measurable functions.*

As an application of this theorem, we have the following proposition which essentially proves the stochastic process associated with the operator (4.33) is the unique solution to the stochastic differential equation (4.34) for a certain choice of M, β, σ and $\mathbf{k}$.

Proposition 4.6.2. *Assume $\mathbf{Z}$ be a solution to the stochastic differential equation (4.34) with $M = \sqrt{\widetilde{\mathbf{D}}}$, matrix σ with entries $\sigma_{ij} = \dfrac{\partial y_j}{\partial \phi_i}$ for $i, j \in \{1, 2, ..., n\}$, the vector $\mathbf{k}$ as defined in (4.30) and $\beta = \dfrac{2\lambda - 1}{2\lambda}$. Then for any $f \in \mathcal{D}_\lambda$*

$$f(\mathbf{Z}_t) - f(\mathbf{Z}_0) - \int_0^t \widehat{\mathcal{L}}_s(f(\mathbf{Z}_s))\ ds \tag{4.35}$$

is a $\widehat{P}$-martingale. Here $\widehat{P}$ is the law of $\mathbf{Z}$.

Proof. The proof of this proposition is a simple application of Peskir's change of variable formula.

$$
\begin{aligned}
f(\mathbf{Z}_t) = f(\mathbf{Z}_0) &+ \sum_{i=1}^{n} \int_0^t \frac{\partial f}{\partial y_i}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-})\ dZ_s^i \\
&+ \frac{1}{2} \sum_{i,j=1}^{n} \int_0^t \frac{\partial^2 f}{\partial y_i \partial y_j}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-})\ d\langle Z^i, Z^j\rangle_s \\
&+ \frac{1}{2} \int_0^t \Big(\frac{\partial f}{\partial y_n}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n+}) - \frac{\partial f}{\partial y_n}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-}) \Big)\ dL_s^{0^+}(\mathbf{Z}) \\
= f(\mathbf{Z}_0) &+ \sum_{i,j=1}^{n} \int_0^t \sqrt{\widetilde{\mathbf{D}}} \sigma_{ij} \frac{\partial f}{\partial y_i}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-})\ dB_s^j \\
&+ \sum_{i=1}^{n} \int_0^t k_i \frac{\partial f}{\partial y_i}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-})\ ds \\
&+ \int_0^t \frac{2\lambda - 1}{2\lambda} \frac{\partial f}{\partial y_n}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-}) dL_t^{0^+}(\mathbf{Z}) \\
&+ \frac{1}{2} \sum_{i,j=1}^{n} \int_0^t \widetilde{\mathbf{D}} a_{ij} \frac{\partial^2 f}{\partial y_i \partial y_j}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-})\ ds \\
&+ \frac{1}{2} \int_0^t \Big(\frac{\partial f}{\partial y_n}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n+}) - \frac{\partial f}{\partial y_n}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-}) \Big)\ dL_s^{0^+}(\mathbf{Z})
\end{aligned}
$$

and since $f \in \mathcal{D}_\lambda$, the local time terms in the last equation cancel each other. Therefore,

$$
\begin{aligned}
f(\mathbf{Z}_t) = f(\mathbf{Z}_0) &+ \sum_{i,j=1}^{n} \int_0^t \sqrt{\widetilde{\mathbf{D}}} \sigma_{ij} \frac{\partial f}{\partial y_i}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-})\ dB_s^j \\
&+ \sum_{i=1}^{n} k_i \frac{\partial f}{\partial y_i}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-})\ ds + \frac{1}{2} \sum_{i,j=1}^{n} \int_0^t \widetilde{\mathbf{D}} a_{ij} \frac{\partial^2 f}{\partial y_i \partial y_j}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-})\ ds \\
= f(\mathbf{Z}_0) &+ \sum_{i,j=1}^{n} \int_0^t \sqrt{\widetilde{\mathbf{D}}} \sigma_{ij} \frac{\partial f}{\partial y_i}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-})\ dB_s^j \\
&+ \int_0^t \Big(\frac{1}{2} \sum_{i,j=1}^{n} a_{ij} \widetilde{\mathbf{D}} \frac{\partial^2 f}{\partial y_i \partial y_j}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-}) + \sum_{i=1}^{n} k_i \frac{\partial f}{\partial y_i}(Z_s^1, ..., \widehat{Y}_s^{n-1}, \widehat{Y}_s^{n-}) \Big)\ ds \\
= f(\mathbf{Z}_0) &+ \sum_{i,j=1}^{n} \int_0^t \sqrt{\widetilde{\mathbf{D}}} \sigma_{ij} \frac{\partial f}{\partial y_i}(Z_s^1, ..., Z_s^{n-1}, Z_s^{n-})\ dB_s^j + \int_0^t \widehat{\mathcal{L}}_s(f(\mathbf{Z}_s))\ ds
\end{aligned}
$$

Hence $f(\mathbf{Z}_t) - f(\mathbf{Z}_0) - \int_0^t \widehat{\mathcal{L}}_s(f(\mathbf{Z}_s))\ ds$ is a $\widehat{P}$-martingale. □

As mentioned in the introduction, proving existence and uniqueness of solutions to stochastic differential equations of the form (4.34) is quite challenging. We relate the solution of (4.34) with another stochastic process which satisfies a SDE with no local time term.

For $\gamma(\mathbf{y}) = \dfrac{1}{2(1-\beta)}\mathbb{I}_{[y_n \geq 0]} + \dfrac{1-2\beta}{2(1-\beta)}\mathbb{I}_{[y_n<0]} = \gamma_1\mathbb{I}_{[y_n\geq 0]} + \gamma_2\mathbb{I}_{[y_n<0]}$, let us consider the following SDE:

$$d\widehat{\mathbf{Z}}_t = \frac{M(\widehat{\mathbf{Z}}_t)}{\gamma(\widehat{\mathbf{Z}}_t)}\ \sigma(\widehat{\mathbf{Z}}_t)d\mathbf{B}_t + \frac{\mathbf{k}(\widehat{\mathbf{Z}}_t)}{\gamma(\widehat{\mathbf{Z}}_t)}dt \tag{4.36}$$

Assuming the existence and uniqueness of solution to SDE 4.36, we now prove the Theorem 4.6.1.

Proof of Theorem 4.6.1. . Let $\widehat{\mathbf{Z}}$ be the unique solution to the SDE (4.36) with conditions on M, σ and $\mathbf{k}$ as given in Theorem 4.6.1. Define a stochastic process

$$\mathbf{Z} = \gamma(\widehat{\mathbf{Z}})\widehat{\mathbf{Z}}. \tag{4.37}$$

Claim: The process defined in (4.37) is indeed the unique solution to the SDE (4.34).

Proof of this claim is a simple application of Peskir's change of variable formula and Itô formula to the stochastic process $\mathbf{Z}$.

Let us denote the right hand side of the equation (4.37) by $\mathbf{h}(\widehat{\mathbf{Z}})$. Then notice that the following calculation yield the relationship between the one sided local time of $\mathbf{h}(\widehat{\mathbf{Z}})$ and $\widehat{\mathbf{Z}}$ at zero.

$$\begin{aligned} L_t^{0^+}(\mathbf{h}(\widehat{\mathbf{Z}})) &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_0^t\ 1_{[0\leq h_n(\widehat{\mathbf{Z}})_s<\epsilon]}\ d\langle h_n(\widehat{\mathbf{Z}}), h_n(\widehat{\mathbf{Z}})\rangle_s \\ &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_0^t\ 1_{[0\leq \gamma_1\widehat{\mathbf{Z}}_s^n<\epsilon]}\gamma_1^2\ d\langle \widehat{Z}^n, \widehat{Z}^n\rangle_s \\ &= \gamma_1 \lim_{\frac{\epsilon}{\gamma_1}\to 0}\frac{\gamma_1}{\epsilon}\int_0^t\ 1_{[0\leq \widehat{Z}_s^n<\frac{\epsilon}{\gamma_1}]}\ d\langle \widehat{Z}^n, \widehat{Z}^n\rangle_s \\ &= \gamma_1\ L_t^{0^+}(\widehat{\mathbf{Z}}). \end{aligned} \tag{4.38}$$

Since for each $j \in \{1, 2, ..., n-1\}$, h_j is C^2, by Itô formula

$$h_j(\widehat{\mathbf{Z}}_t) = h_j(\widehat{\mathbf{Z}}_0) + \int_0^t \gamma_1 d\widehat{Z}_s^j$$

Now denote $\widetilde{\mathbf{Z}} = (\widehat{Z}^1, \widehat{Z}^2, ..., \widehat{Z}^{n-1})$. For h_n, Peskir's change of variable formula gives

$$\begin{aligned} h_n(\widehat{\mathbf{Z}}_t) &= h_n(\widehat{\mathbf{Z}}_0) + \sum_{i=1}^{n} \int_0^t \frac{\partial h_n}{\partial z_i}(\widetilde{\mathbf{Z}}_s, \widehat{Z}_s^{n-})\ d\widehat{Z}_s^i + \frac{1}{2} \sum_{i,j=1}^{n} \int_0^t \frac{\partial^2 h_n}{\partial z_i \partial z_j}(\widetilde{\mathbf{Z}}_s, \widehat{Z}_s^{n-})\ d\langle \widehat{Z}^i, \widehat{Z}^j \rangle_s \\ &\quad + \frac{1}{2} \int_0^t \Big(\frac{\partial h_n}{\partial z_n}(\widetilde{\mathbf{Z}}_s, \widehat{Z}_s^{n+}) - \frac{\partial h_n}{\partial z_n}(\widetilde{\mathbf{Z}}_s, \widehat{Z}_s^{n-}) \Big)\ dL_s^{0^+}(\widehat{\mathbf{Z}}) \\ &= h_n(\widehat{\mathbf{Z}}_0) + \int_0^t \gamma\ d\widetilde{Z}_s^n + \frac{1}{2} \int_0^t (2\gamma_1 - 1)\ dL_s^{0^+}(\widehat{\mathbf{Z}}) \\ &= h_n(\widehat{\mathbf{Z}}_0) + \int_0^t \gamma\ d\widehat{Z}_s^n + \int_0^t \frac{2\gamma_1 - 1}{2\gamma_1}\ dL_s^{0^+}(\mathbf{h}(\widehat{\mathbf{Z}})) \end{aligned}$$

where the last equation is using (4.38).

Thus we have

$$d\mathbf{h}(\widehat{\mathbf{Z}}_t) = M(\mathbf{h}(\widehat{\mathbf{Z}}_t))\ \sigma(\mathbf{h}(\widehat{\mathbf{Z}}_t)) d\mathbf{B}_t + \mathbf{k}(\mathbf{h}(\widehat{\mathbf{Z}}_t)) dt + \begin{pmatrix} 0 \\ . \\ . \\ . \\ 0 \\ \beta\ dL_t^{0^+}(\mathbf{h}(\widehat{\mathbf{Z}})) \end{pmatrix}$$

Thus $\mathbf{Z}$ given in (4.37) is the unique solution to the SDE (4.34) with conditions on M, σ, $\mathbf{k}$ and β as given in Theorem 4.6.1.

□

Now using the Feynman-Kac formula we get the stochastic process associated with the operator $\mathcal{L}_{\mathbf{y}}$ given in (4.32) or the PDE with interface conditions (4.28). The following proposition gives us the result.

Proposition 4.6.3. *For a fixed time $t \geq 0$ and $\mathbf{Z}$ defined in (4.37), define an exponential random variable τ such that*

$$P(\tau > t \mid \mathbf{Z}_s,\ 0 \leq s \leq t) = \exp\Big\{ - \int_0^t r(Y_u) du \Big\}$$

Define

$$\mathbf{Y}_t = \begin{cases} \mathbf{Z}_t & \textit{if} \;\; t < \tau \\ \infty & \textit{if} \;\; t \geq \tau. \end{cases}$$

Then $\mathbf{Y}_t$ *is the unique stochastic process associated with the PDE and interface conditions given in (4.28).*

This proposition proves our main theorem Theorem 4.1.2.

It remains to show the existence and uniqueness of solutions to SDE given in (4.36). Existence of a unique solution to this SDE is not quite obvious as its coefficients are discontinuous. We will established the unique solution step by step using following corollaries.

Assume that the matrix $\mathbf{a} = (a_{ij})$ is uniformly positive definite and a_{ij}'s are bounded continuous functions. Define the differential operator

$$\mathcal{L}^{(1)} = \frac{1}{2}\sum_{i,j=1}^{n} a_{ij}(\cdot)\frac{\partial^2}{\partial y_i \partial y_j} \tag{4.39}$$

acting on functions in $C^2(\mathbb{R}^n)$. Then from Lemma 4.2.5 there is a unique probability measure $P^{(1)}$ that solves the martingale problem associated with $\mathcal{L}^{(1)}$. Moreover, the stochastic process associated with the operator can be written uniquely as $\mathbf{Y}_t^{(1)} = y^{(1)} + \int_0^t \sigma(\mathbf{Y}_s^{(1)}) d\mathbf{B}_s$, where $\mathbf{B}$ is n dimensional Brownian motion and $\sigma\sigma^T = \mathbf{a}$.

Let $P^{(2)}$ be the probability measure satisfying the following Radon-Nicodym derivative

$$\frac{dP^{(2)}}{dP^{(1)}} = \exp\Bigg\{\int_0^t \langle \mathbf{a}^{-1}\frac{\gamma(\mathbf{Y}_u^{(1)})\mathbf{k}(\mathbf{Y}_u^{(1)})}{M^2(\mathbf{Y}_u^{(1)})}, d\mathbf{Y}_u^{(1)}\rangle - \frac{1}{2}\int_0^t \langle \frac{\gamma(\mathbf{Y}_u^{(1)})\mathbf{k}(\mathbf{Y}_u^{(1)})}{M^2(\mathbf{Y}_u^{(1)})}, \mathbf{a}^{-1}\frac{\gamma(\mathbf{Y}_u^{(1)})\mathbf{k}(\mathbf{Y}_u^{(1)})}{M^2(\mathbf{Y}_u^{(1)})}\rangle du\Bigg\} \tag{4.40}$$

where $\mathbf{a} = (a_{ij})$ is as defined in (4.39), $\mathbf{k}$ is bounded measurable function, M positive piecewise constants in $y_n \geq 0$ and $y_n < 0$, and γ is as defined in (4.36). Since $\mathbf{a}$ is uniformly positive definite and $\frac{\gamma\mathbf{k}}{M^2}$ is bounded measurable, this Radon-Nicodym derivative exists by Theorem 7.2.2 in Stroock and Varadhan (1979).

Now define a differential operator $\mathcal{L}^{(2)}$ acting on functions in $C^2(\mathbb{R}^n)$ as follows:

$$\mathcal{L}_t^{(2)} = \frac{1}{2}\sum_{i,j=1}^{n} a_{ij}(t,\cdot)\frac{\partial^2}{\partial y_i \partial y_j} + \sum_{j=1}^{n}\frac{\gamma(\cdot)k_j(t,\cdot)}{M^2(\cdot)}\frac{\partial}{\partial y_j} \tag{4.41}$$

Corollary 4.6.4. *The probability measure $P^{(2)}$ defined in (4.40) is the unique probability measure that solves the martingale problem associated with the operator $\mathcal{L}_t^{(2)}$ defined in (4.41). Moreover, the stochastic process associated with the operator can be written uniquely as $\mathbf{Y}_t^{(2)} = y^{(2)} + \int_0^t \sigma(\mathbf{Y}_s^{(2)})d\mathbf{B}_s + \int_0^t \frac{\gamma(\mathbf{Y}_s^{(2)})\mathbf{k}(\mathbf{Y}_s^{(2)})}{M^2(\mathbf{Y}_s^{(2)})}ds$, where $\mathbf{B}$ is n dimensional Brownian motion.*

Proof. From the Theorem 5:11 on page 118 of Stroock (1987), the martingale problem associated to $\mathcal{L}^{(2)}$ is well-posed. From Theorem 7.2.2 on page 188 of Stroock and Varadhan (1979), one has the probability measure $P^{(2)}$ in terms of Radon-Nicodym derivative. Also associated stochastic process is given by the Theorem 6.2 on page 91 of Stroock (1987). □

Now that we have the existence and uniqueness of the solutions to martingale problem associated with the operator $\mathcal{L}^{(2)}$, we use the random time change discussed in Section 4.3 to prove existence and uniqueness of the solutions to martingale problem associated with the following operator acting on function in $C^2(\mathbb{R}^n)$.

$$\mathcal{L}_t^{(3)} = \frac{1}{2}\sum_{i,j=1}^{n} \frac{M^2(t,\cdot)}{\gamma^2(\cdot)}\, a_{ij}(t,\cdot)\frac{\partial^2}{\partial y_i \partial y_j} + \sum_{j=1}^{n}\frac{k_j(t,\cdot)}{\gamma(t,\cdot)}\frac{\partial}{\partial y_j} \tag{4.42}$$

where a_{ij}, k_j, M and γ are defined as in (4.41).

Define a bounded, measurable and uniformly positive function φ on $\mathbb{R}^n$ such that for $\mathbf{y} = (y_1, y_2, ..., y_n) \in \mathbb{R}^n$,

$$\varphi(\mathbf{y}) = \frac{M^2(\mathbf{y})}{\gamma^2(\mathbf{y})} \tag{4.43}$$

Also define $\tau_\varphi : [0,\infty) \times \Omega \to [0,\infty)$ such that for each continuous function $\omega \in \Omega$ and for $t \geq 0$,

$$\int_0^{\tau_\varphi(t,\omega)} \frac{1}{\varphi(\mathbf{Y}^{(2)}(u,\omega))} du = t \tag{4.44}$$

where φ is as defined in (4.43).

Now define a function S_φ determine by $\mathbf{Y}^{(2)}$ as follows:

$$S_\varphi : \Omega \to \Omega \quad \text{such that} \quad \mathbf{Y}^{(2)}(t, S_\varphi(\omega)) = \mathbf{Y}^{(2)}(\tau_\varphi(t,\omega),\omega). \tag{4.45}$$

Corollary 4.6.5. *The probability measure $P^{(3)} = P^{(2)} \circ S_\varphi^{-1}$, where S_φ is as define in (4.45), is the unique probability measure that solves the martingale problem associated with the operator $\mathcal{L}^{(3)}$ defined in (4.42). Moreover, the unique stochastic process $\mathbf{Y}^{(3)}$, associated with the operator (4.42) is the solution to*

$$d\widehat{\mathbf{Z}}_t = \frac{M(\widehat{\mathbf{Z}}_t)}{\gamma(\widehat{\mathbf{Z}}_t)}\, \sigma(\widehat{\mathbf{Z}}_t) d\mathbf{B}_t + \frac{\mathbf{k}(\widehat{\mathbf{Z}}_t)}{\gamma(\widehat{\mathbf{Z}}_t)} dt. \tag{4.46}$$

Proof. From Corollary 4.6.4, we have that $P^{(2)}$ solves the martingale problem for $\mathbf{a}$ and $\frac{\gamma \mathbf{k}}{M^2}$ (or associated with $\mathcal{L}^{(2)}$). Then by Theorem 6.5.2 on page 159 of Stroock and Varadhan (1979), $P^{(2)} \circ S_\varphi^{-1}$ solves the martingale problem for $\varphi(\cdot)\mathbf{a}(\cdot)$ and $\varphi(\cdot)\dfrac{\gamma(\cdot)\mathbf{k}(\cdot)}{M^2(\cdot)}$. Furthermore, since $P^{(2)}$ is unique from Corollary 4.6.4, $P^{(2)} \circ S_\varphi^{-1}$ is unique from Theorem 6.5.4 on page 160 of Stroock and Varadhan (1979). Now notice that $\varphi(\cdot)\mathbf{a}(\cdot) = \frac{M^2(\cdot)}{\gamma^2(\cdot)}\mathbf{a}(\cdot)$, $\varphi(\cdot)\frac{\gamma(\cdot)\mathbf{k}(\cdot)}{M^2(\cdot)} = \frac{\mathbf{k}(\cdot)}{\gamma(\cdot)}$ and the differential operator associated with them is $\mathcal{L}^{(3)}$.

Now denote $\hat{\sigma} = \frac{M}{\gamma}\, \sigma$. Then it is clear that $\hat{\sigma}\hat{\sigma}^t = \frac{M^2}{\gamma^2}\sigma\sigma^t = \frac{M^2}{\gamma^2}\mathbf{a} = \varphi\mathbf{a}$.

We have that $P^{(2)} \circ S_\varphi^{-1}$ is the unique solution to the martingale problem associated to $\mathcal{L}^{(3)}$. Then from Theorem 2.6 on page 91 of Stroock book: given a measurable $\hat{\sigma} : \mathbb{R}^n \longrightarrow \text{Hom}(\mathbb{R}^n;\mathbb{R}^n)$ satisfying $\varphi\mathbf{a} = \hat{\sigma}\hat{\sigma}^t$, there is a n-dimensional Brownian motion $\mathbf{B}_t$ on some probability space $(\Omega, \mathcal{F}, Q)$ and a continuous $\{\mathcal{F}_t\}$-progressively measurable function $\mathbf{Y}^{(3)} : [0.\infty) \times \Omega \longrightarrow \mathbb{R}^n$ s.t.

$$\mathbf{Y}_t^{(3)} = y^{(3)} + \int_0^t \hat{\sigma}(\mathbf{Y}_s^{(3)})d\mathbf{B}_s + \int_0^t \varphi(\mathbf{Y}_s^{(3)})\mathbf{k}(\mathbf{Y}_s^{(3)})ds \quad \text{for} \ \ t \geq 0$$

(a.s., Q) and $P^{(2)} \circ S_\varphi^{-1} = Q \circ (\mathbf{Y}_\cdot^{(3)})^{-1}$. Since $P^{(2)} \circ S_\varphi^{-1}$ is unique, Q is also unique. The result is immediate by just noticing that $\hat{\sigma} = \frac{M}{\gamma}\ \sigma$ and $\varphi \frac{\gamma \mathbf{k}}{M^2} = \frac{\mathbf{k}}{\gamma}$.

This proves the existence and uniqueness of the solutions to the SDE defined in (4.36).

□

4.7 Stochastic process for the diffusion equation in radially symmetric domain with interface on a sphere

Here we consider an example of a diffusion problem when the diffusion coefficient is piecewise constant across a sphere centered at the origin. This makes this sphere an interface to the problem. We assume that the initial data is radially symmetric in $\mathbb{R}^n$.

Without loss of generality assume that the interface is a sphere $\mathcal{S}$, centered at zero with radius one. Denote $\mathcal{A}_1$ be the inside of $\mathcal{S}$ and $\mathcal{A}_2 = \mathbb{R}^n \setminus \bar{\mathcal{A}}_1$. Let c be a real valued function in $C^{1,2}([0, \infty), \mathbb{R}^n)$ such that it satisfies the diffusion equation,

$$\frac{\partial c}{\partial t} = \frac{1}{2} \nabla \cdot \big(\mathbf{D} \nabla c\big), \quad c(0, \mathbf{x}) = c_0 \tag{4.47}$$

with the interface condition

$$\Big[\bar{\lambda} \frac{\partial c}{\partial \eta}\Big] = 0, \quad [c] = 0 \tag{4.48}$$

where η is the outward normal to the sphere $\mathcal{S}$, $\mathbf{D}(\mathbf{x}) = D_1 \mathbb{I}_{[\mathbf{x} \in \mathcal{A}_1]} + D_2 \mathbb{I}_{[\mathbf{x} \in \mathcal{A}_2]}$ and $\bar{\lambda}(\mathbf{x}) = (1 - \lambda)\mathbb{I}_{[\mathbf{x} \in \mathcal{A}_1]} + (\lambda)\mathbb{I}_{[\mathbf{x} \in \mathcal{A}_2]}$. We also assume c_0 is radially symmetric in $\mathbb{R}^n$.

Since c_0 is radially symmetric, we have that the solution c of the equation (4.47) with the interface conditions (4.48) is also radially symmetric in $\mathbb{R}^n$. Thus we have (4.47) and (4.48) in spherical coordinates

$$\frac{\partial c}{\partial t} = \frac{1}{2r^2}\frac{\partial}{\partial r}\Big(\mathbf{D}r^2\frac{\partial c}{\partial r}\Big) \tag{4.49}$$

$$\Big[\bar{\lambda}r^2\frac{\partial c}{\partial r}\Big] = 0, \quad [c] = 0 \quad \text{at} \quad r = 1 \tag{4.50}$$

with $\mathbf{D}(r) = D_1\mathbb{I}_{[r\leq 1]} + D_2\mathbb{I}_{[r>1]}$ and $\bar{\lambda}(r) = (1-\lambda)\mathbb{I}_{[r\leq 1]} + \lambda\mathbb{I}_{[r>1]}$.

Our aim in this section is to find the stochastic process associated with the equation (4.49) and conditions (4.50). We first identify the stochastic differential equation associated with them. For that it is helpful to write our equation (4.49) as follows:

$$\frac{\partial c}{\partial t} = \frac{\mathbf{D}}{2}\frac{\partial^2 c}{\partial r^2} + \frac{\mathbf{D}}{r}\frac{\partial c}{\partial r}$$

Let us consider the following stochastic differential equation.

$$dR_t = \sqrt{\mathbf{D}}dB_t + \frac{\mathbf{D}}{R_t}dt + \frac{2\lambda - 1}{2\lambda}dL_t^{1^+}(R) \tag{4.51}$$

In Le Gall (1982), he proves the existence and uniqueness of solutions to the SDE of the form (4.51). That being said, we state our main result as follows.

Proposition 4.7.1. *Let R be the unique solution of the stochastic differential equation (4.51). Then R is the stochastic process associated with the equation (4.49) with conditions (4.50).*

Proof. The proof of this proposition is a simple application of Itô-Tanaka formula.

Let f be a real valued function in $C^1(\mathbb{R})\cap C^2(\mathbb{R}\backslash\{1\})$ such that $(1-\lambda)f'_-(1) = \lambda f'_+(1)$ and with the second generalized derivative is given by $f''(da) = f''(a)da + \big[f'_+(1) - f'_-(1)\big]\delta_1$.

Then from Itô-Tanaka formula,

$$\begin{aligned}
f(R_t) - f(R_0) &= \int_0^t f'_-(R_s)dR_s + \frac{1}{2}\int_{\mathbb{R}} L_t^{a^+}(R)f''(da) \\
&= \int_0^t f'_-(R_s)\sqrt{\mathbf{D}}dB_s + \int_0^t f'_-(R_s)\frac{\mathbf{D}}{R_s}ds + \int_0^t f'_-(R_s)\frac{2\lambda-1}{2\lambda}dL_s^{1^+}(R) \\
&\quad + \frac{1}{2}\int_0^t f''(R_s)d\langle R,R\rangle_s + \frac{1}{2}\big[f'_+(1) - f'_-(1)\big]L_t^{1^+}(R) \\
&= \int_0^t f'_-(R_s)\sqrt{\mathbf{D}}dB_s + \int_0^t f'_-(R_s)\frac{\mathbf{D}}{R_s}ds + \frac{1}{2}\int_0^t f''(R_s)\mathbf{D}ds \\
&\quad + f'_-(1)\frac{2\lambda-1}{2\lambda}L_t^{1^+}(R) + \frac{1}{2}\Big(\frac{1-2\lambda}{\lambda}\Big)f'_-(1)L_t^{1^+}(R) \\
&= \int_0^t f'_-(R_s)\sqrt{\mathbf{D}}dB_s + \int_0^t \Big(\frac{\mathbf{D}}{2}f''(R_s) + \frac{\mathbf{D}}{R_s}f'_-(R_s)\Big)ds
\end{aligned}$$

Thus we have $f(R_t) - f(R_0) - \int_0^t \Big(\frac{\mathbf{D}}{2}f''(R_s) + \frac{\mathbf{D}}{R_s}f'_-(R_s)\Big)ds$ is a martingale. This proves the proposition. □

4.8 Skorokhod Problem

The Skorokhod problem was originally introduced in Skorokhod (1961) in order to study continuous solutions to stochastic differential equations with a reflecting boundary. Before giving the definition of the Skorokhod problem let us first introduce some notation. We denote the continuous $\mathbb{R}^n$ valued function defined on $[0,\infty)$ by $C([0,\infty);\mathbb{R}^n)$ and denote the $\mathbb{R}^d$ valued functions of bounded variation on the set $[0,T]$ by $BV([0,T];\mathbb{R}^n)$. Also we denote the total variation of a function $f:[0,T]\to\mathbb{R}^n$ by $|f|$.

Definition 4.8.1 (Skorokhod Problem)**.** *Let $\mathcal{O}$ be a domain in $\mathbb{R}^d$. Let Γ be the collection of unit outward normal to $\partial\mathcal{O}$. Then for a given $\mathbf{W}\in C([0,\infty);\mathbb{R}^n)$ with $\mathbf{W}_0\in\bar{\mathcal{O}}$, we say the pair $(\mathbf{X},\mathbf{k})$ with $\mathbf{X}\in C([0,\infty);\mathbb{R}^n)$ and $\mathbf{k}\in BV([0,T];\mathbb{R}^n)$ for all $T<\infty$ satisfy the Skorokhod problem for $\mathbf{W}$ if the following two conditions are satisfied,*

i. $\mathbf{X}_t = \mathbf{W}_t + \mathbf{k}_t$ *for* $t\geq 0$, *ii.* $\mathbf{k}_t = \int_0^t \eta(\mathbf{X}_s) d|\mathbf{k}|_s$ *where* $\eta \in \Gamma$ *and* $|\mathbf{k}|_t = \int_0^t \mathbb{I}_{[\mathbf{X}_s \in \partial\mathcal{O}]} d|\mathbf{k}|_s$ *for* $t \geq 0$.

It is well known that if $\mathcal{O} = [0, \infty)$, W is one dimensional Brownian motion and $k_t = \sup_{0 \leq s \leq t} -W_s \vee 0$, the process X given by the Skorokhod problem is reflected Brownian motion reflected at zero; for example see Skorokhod (1961).

Existence of weak solutions to Skorokhod problem in a smooth domain $\mathcal{O}$ is proved by Stroock and Varadhan (1971). For the case of the convex domain is treated in Tanaka (1979). Later in Lions and Sznitman (1984), it was proved the existence of solutions to the Skorokhod problem with an oblique reflecting boundary conditions.

We believe that Skorokhod problem can be extended for the case of partial reflecting boundary condition. That being said, this would help one to formulate the Skorokhod problem in the following manner so that its solution can be used to connect with the stochastic process associated with diffusion problems with interfaces having general geometries.

Let $\mathcal{O}$ be a smooth bounded domain in $\mathbb{R}^n$. Denote the n-dimension Brownian motion by $\mathbf{B}$ and for any $\mathbf{x}' \in \partial\mathcal{O}$, denote the unit normal pointing into $\mathcal{O}^c$ at $\mathbf{x}'$ by $\eta(\mathbf{x}')$. Also suppose $0 < \alpha(\mathbf{x}') < 1$ for all $\mathbf{x}' \in \partial\mathcal{O}$.

Now find the pair $(\mathbf{X}, \mathbf{k})$ satisfying the following Skorokhod problem with an additional third condition.

i. $d\mathbf{X}_t = d\mathbf{B}_t + \eta(\mathbf{X}_t) d\mathbf{k}_t$,

ii. $\mathbf{k}$ is of bounded variation, increases only at times when $\mathbf{X}$ is at $\partial\mathcal{O}$,

iii. for any $\mathbf{x}' \in \partial\mathcal{O}$,

$$\alpha(\mathbf{x}') \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_0^t \mathbb{I}_{[0 \leq (\mathbf{X}_s - \mathbf{x}') \cdot \eta(\mathbf{x}') < \epsilon]} ds = (1 - \alpha(\mathbf{x}')) \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_0^t \mathbb{I}_{[-\epsilon < (\mathbf{X}_s - \mathbf{x}') \cdot \eta(\mathbf{x}') < 0]} ds$$

5 GENERAL CONCLUSIONS AND FUTURE WORK

This thesis studies a class of stochastic processes and their association with parabolic equations having discontinuous coefficients that arise from models of physical problems. One of the important aspects of these parabolic equations considered in this thesis is the presence of an interface condition.

In the first part, we provide new theoretical results for functionals of skew Brownian motion and its associated PDE, together with an application to advection-dispersion across a sharp interface. Trivariate density of skew Brownian motion, the position, occupation and local times; probability density function of skew Brownian motion with drift and the first passage time density formula for skew Brownian motion are some of the new results presented in this part.

The second part provides a mathematical treatment of solute transport when the mean velocity is perpendicular to a sharp interface. The results presented in this part extend the results of Ramirez et al. (2008) to the case of Fickian convection-dispersion for solute transport in the direction of flow orthogonal to a sharp interface. Also, this part provides specific results to explain the interesting types of symmetries and asymmetries in the breakthrough curves, concentration curves and occupation times of a conservative tracer across an sharp interface recently reported by Berkowitz et al. (2009).

The third part provides the existence and uniqueness of stochastic processes associated with more general class of parabolic equations with discontinuous coefficients that are of mathematical interest. The geometry of the interface studied in this chapter is a graph of a function and the condition at the interface is also general. One of the important results provided in this chapter is the existence and uniqueness of solutions to a general stochastic differential equation with a local time term in higher dimension of the form (4.34).

During the process of preparation of this work many interesting questions were raised and a lot of them remain unsolved. Following are some of the more important open problems and avenues of research that is believed to be worthwhile following.

The solution to diffusion equation with the planar interface is not known when the coefficients of the interface condition depends on the position. To answer this case, development of a variably skewed Brownian motion, where the skewness parameter is a function, might be a useful tool.

The analysis of existence and uniqueness of stochastic processes associated with parabolic equations with interfaces on general geometry is of great value in applications of physical problems. For the case of piecewise constant coefficients, this would be the natural extension of the results presented in third part. One big problem that stands in the way is the lack of understanding of the local time defined on surfaces and lack of machinery to connect the PDE with its associated stochastic differential equation. At the end of the third part it is conjectured that this general interface problem can be solved by formulating a Skorohod problem. Again in there, one should understand the process of bounded variation.

Also the other important extension one could study is the extension of Martingale problem for differential operators acting on functions that are not C^2.

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