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Abstract

This paper is a follow-up to Dean and Russell[2] in which the formulation of our model of NAPL flow in heterogeneous porous media is based on the traditional argument of developing a Fokker-Planck equation for a diffusion process and then modifying this equation to handle the behavior of the fluid particle at an interface between sands of different permeabilities. Since the capillary diffusivity can change significantly across the interface, we call these changes jumps and incorporate them into the stochastic differential equation that describes the motion of the NAPL particle. Since this is a traditional approach that is modified to incorporate non-traditional behavior such as jumps, we call it a bottom-up approach. The modified stochastic differential equation can then model pooling and channeling that occurs at such interfaces. In this paper, an attempt is made to accomplish the same result starting with a theory of stochastic processes that allows jumps. We start with semimartingale processes which are càdlàg. Since these processes allow jumps by definition, we call this approach the top-down approach.

1 Introduction

The objective of the next few pages is to use some of the semimartingale theory that can be found in Protter[4, 5] to justify from a top down perspective the stochastic differential equation description of a DNAPL or LNAPL particle trajectory in heterogeneous porous media. The stochastic differential equation is given in Dean and Russell[2] as Equation[17], or in a slightly different form as Equation[3], below. We assume that the behavior of the DNAPL or LNAPL particle can be described as a semimartingale whose sample paths almost surely experience only a finite number of bounded jumps over the time interval of interest. The domain of the problem is subdivided into computational cells that consist of homogeneous material and whose boundaries coincide with the boundaries of heterogeneous areas of the general domain. An example of this is shown in Figure 1, below. As long as the particle in in the interior of a computational cell, it will experience a convected diffusion. However, when the particle encounters the interface between two computational of different permeabilities, it will be subjected to an instantaneous change in the capillary diffusivity. It is this instantaneous change in the capillary diffusivity that we call a *jump*. If the particle is moving from a computational cell with coarse sand (or higher permeability) to a computational cell containing fine sand (or lower permeability), then the NAPL will pool at the interface. The NAPL will continue to pool at the interface until its saturation along the interface is great enough so that (based on the Brooks-Corey theory) the capillary pressure in the coarse sand exceeds the entry pressure of the fine sand. Section 8 in Dean and Russell[2] gives some formulations for computing the NAPL saturations and Section 10 discusses the capillary end effect and how it applies to this problem.

As in Dean and Russell[2] the justification of the top down perspective begins with the Itô formula, and this time it will be a version that applies to semimartingales. Since semimartingales are càdlàg processes, they can have jumps.

2 Itô's Formula

Suppose that $X^1, \cdots, X^d$ are càdlàg semimartingales, then the quadratic covariation of X^j, X^k, $1 \leq j, k \leq d$ is given by, Protter[5],

$$[X^j, X^k]_t = [X^j, X^k]_t^c + \sum_{s \leq t} \Delta X_s^j \Delta X_s^k \tag{1}$$

where $\sum_{s\le t}\Delta X_s^j\Delta X_s^k$ represents the jump part of $[X^j,X^k]_t$, and Itô's formula is given by the following:

Theorem: (Itô) Let $X^1,X^2,\cdots,X^d$ be semimartingales and let $f\in C^{1,2}\left([0,\infty)\times\Re^d\right)$. Then if $\vec{X}_t=(X_t^1,\cdots,X_t^d)^{\mathsf{T}}$,

$$\begin{aligned} f(t,\vec{X}_t) &= f(0,\vec{X}_0)+\int_0^t f_t(s,\vec{X}_s)\,ds+\sum_{i=1}^d\int_0^t f_j(s,\vec{X}_{s-})\,dX_s^j \\ &+ \frac{1}{2}\sum_{j=1}^d\sum_{k=1}^d\int_0^t f_{jk}(s,\vec{X}_{s-})\,d[X^j,X^k]_s \\ &+ \sum_{0<s\le t}\left\{f(s,\vec{X}_s)-f(s,\vec{X}_{s-})-\sum_{j=1}^d f_j(s,\vec{X}_{s-})\Delta X_s^j\right. \\ &- \left.\frac{1}{2}\sum_{j=1}^d\sum_{k=1}^d f_{jk}(s,\vec{X}_{s-})\,(\Delta X_s^j)(\Delta X_s^k)\right\} \end{aligned} \tag{2}$$

The last two lines of this equation represent the jumps in the corresponding terms in the first two lines. Since X^i, $i=1,\cdots,d$ are semimartingales, they are càdlàg so that

$$\Delta X_t^i=X_t^i-X_{t-}^i$$

represents the jump in X^i at t. I think it is important to note that X depends on the pair $(t,\omega)\in[0,\infty)\times\Omega$. So, if ω is fixed at, say $\hat{\omega}$, then $X_t(\hat{\omega})$ is a sample path. If ω is not fixed, then $X_t(\omega)$ is a process. Hence, $\Delta X_t(\omega)=X_t(\omega)-X_{t-}(\omega)$, $\omega\in\Omega$, is a process. In this regard, $[X^j,X^k]^c$ represents the path by path continuous part of $[X^j,X^k]$.

Fluid particle control at a material interface is accomplished using the jump in capillary diffusivity across the interface and the retention functions. The jump in the capillary diffusivity causes the DNAPL to pool on the coarse sand side until the entry pressure of the fine sand is exceeded. If the heterogeneous domain of the problem is subdivided into computational cells of uniform material as illustrated in Figure 1, then the tensor $\mathbf{D}$ will be constant on a cell during a given time step. But, if two adjecent cells contain different material, then $\mathbf{D}$ will have a jump across the boundary between the cells. In one-dimension, $\mathbf{D}$ will have the appearance of a Heaviside step function. The derivative $\nabla^{\mathsf{T}}\mathbf{D}^{\mathsf{T}}$ will then be zero on either side of the boundary and experience a jump at the boundary. Using symbolic derivatives, that jump will have the form of a δ-function. Therefore, $\int_0^t\nabla^{\mathsf{T}}\mathbf{D}^{\mathsf{T}}\,ds=-[[\mathbf{D}]]\vec{n}^+\,\delta(\sigma)$, where σ represents the boundary between the two computational cells, (See Dean and Russell[2], Appendix A). Of course, the particle may experience several such jumps over the course of its total trajectory. Thus, the stochastic differential equation can be written in the form

$$\begin{aligned} \vec{X}_t=\vec{X}_0 &+ \int_0^t\left(\frac{1}{\theta_n}\left(\bar{\lambda}\gamma_n\mathbf{k}\vec{z}-\bar{\lambda}\gamma_w\mathbf{k}\vec{z}+f_n\vec{q}_t\right)\right)\,ds \\ &+ \int_0^t\mathbf{B}(s,\vec{X}_s)\,d\vec{W}_s+\vec{J}(t) \end{aligned} \tag{3}$$

where in this equation, γ_α is the specific weight of the α-phase, $\bar{\lambda}=\frac{\lambda_w\lambda_n}{\lambda_w+\lambda_n}$, $f_n=\frac{\lambda_n}{\lambda_w+\lambda_n}$, $\lambda_\alpha=\frac{k_{r\alpha}}{\mu_\alpha}$, $\vec{z}=(0,0,-1)^{\mathsf{T}}$, μ_α is the viscosity of the α-phase and $\vec{J}(t)$ is determined by the capillary end effect (See Dean and Russell[2], Equation[27] and the accompanying discussion). When the particle is in

the interior of a computational cell, it will experience a convected diffusion. As it moves between computational cells of different material, it will experience a jump.

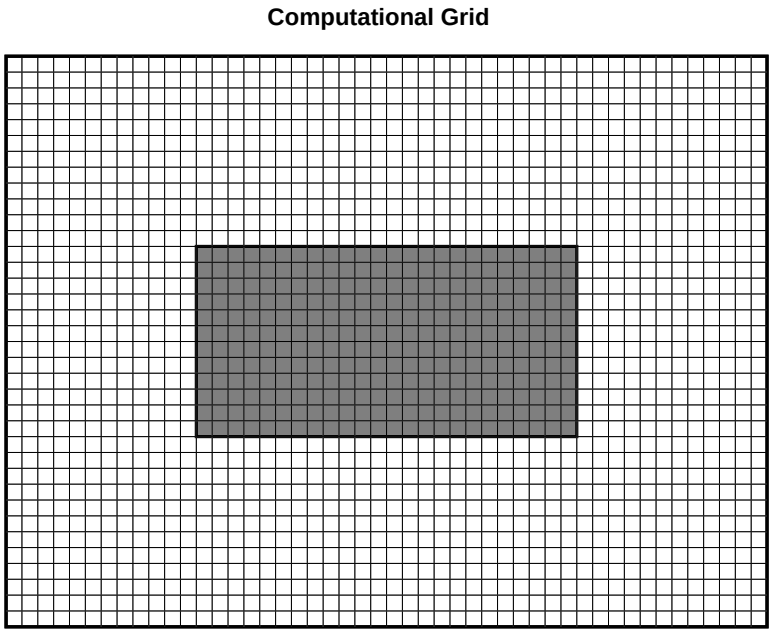

Figure 1: Material Interface

The tensor $\mathbf{D}$ is given by

$$\mathbf{D} = \frac{\bar{\lambda}\mathbf{k}}{n}\frac{dp_c}{dS_n} \tag{4}$$

and $\mathbf{B}$ is derived from $\mathbf{D}$ by

$$2\mathbf{D} = \mathbf{B}\,\mathbf{B}^{\mathsf{T}}$$

In Equation[3], the term $\vec{J}(t)$ represents the jump part of the process and the remainder a convected diffusion. As long as the particle is in a computational cell containing a uniform material, it is governed by the process

$$\begin{aligned}\vec{X}_t = \vec{X}_0 \quad &+ \quad \int_0^t \left(\frac{1}{\theta_n}\left(\bar{\lambda}\gamma_n\mathbf{k}\vec{z} - \bar{\lambda}\gamma_w\mathbf{k}\vec{z} + f_n\vec{q}_t\right)\right)\,ds \\ &+ \quad \int_0^t \mathbf{B}(s,\vec{X}_s)\,d\vec{W}_s \end{aligned} \tag{5}$$

which is the continuous part of the process. The continuous part of a semimartingale can be identified, Protter[5], if it is assumed for the given semimartingale X that

$$\sum_{0<s\leq t} |\Delta X_s| < \infty, \quad \text{a.s. each } \; t > 0 \tag{6}$$

In our case, Equation[3] satisfies this condition because the jumps are all finite and there are only a finite number of them. So, if X is a semimartingale and satisfies Condition[6], then the sum of the jumps is given by

$$J_t = \sum_{0\leq s\leq t} \Delta X_s$$

and by Condition[6] J is a finite variation process. By the Theorem on page 21, J is also a semimartingale. Furthermore, $Y_t = X_t - J_t$ is a continuous semimartingale and by the definition of J_t, $Y_0 = 0$. Then Y has the unique decomposition

$$Y = M + A$$

where M is a continuous local martingale, A is a continuous finite variation process and $M_0 = A_0 = 0$. The decomposition is unique because of Condition[6] and Theorem 31 of Protter[5] which says that Y is a special semimartingale which makes the decomposition unique (See Protter[5], page 129). The process M is then the continuous local martingale part of X, written $X^c = M$.

The jump terms in Equation[2] are given by the following:

$$\sum_{0<s\leq t} \left\{ f(s, \vec{X}_s) - f(s, \vec{X}_{s-}) \right\} \tag{7}$$

$$- \sum_{0<s\leq t} \sum_{j=1}^{d} f_j(s, \vec{X}_{s-}) \Delta X_s^j \tag{8}$$

$$- \sum_{0<s\leq t} \frac{1}{2} \sum_{j=1}^{d} \sum_{k=1}^{d} f_{jk}(s, \vec{X}_{s-}) \, (\Delta X_s^j)(\Delta X_s^k) \tag{9}$$

By moving Equation[7] to the LHS of Equation[2], the finite number of bounded jumps are subtracted out of $f(t, \vec{X}_t)$ leaving the part of $f(t, \vec{X}_t)$ based on the convected diffusion in the interior of the computational cell. Within the computational cell, we can write $X = X^c$ as the continuous part of X.

Similarly, Equation[9] can be combined with the second line of Equation[2] using Equation[1] to give

$$\frac{1}{2} \sum_{j=1}^{d} \sum_{k=1}^{d} \int_0^t f_{jk}(s, \vec{X}_{s-}) \, d[X^j, X^k]_s^c$$

Finally, Equation[8] is combined with the last term in the first line of Equation[2]. Equation[2] becomes

$$\begin{aligned} f(t, \vec{X}_t) &= f(0, \vec{X}_0) + \int_0^t f_t(s, \vec{X}_s) \, ds \\ &+ \sum_{j=1}^{d} \int_0^t f_j(s, \vec{X}_{s-}) \, dX_s^j - \sum_{0<s\leq t} \sum_{j=1}^{d} f_j(s, \vec{X}_{s-}) \, \Delta X_s^j \\ &+ \frac{1}{2} \sum_{j=1}^{d} \sum_{k=1}^{d} \int_0^t f_{jk}(s, \vec{X}_{s-}) \, d[X^j, X^k]_s^c \end{aligned} \tag{10}$$

In keeping with Dean and Russell[2], Equation[17], we assume that the the jumps in the stochastic differential equation describing $\vec{X}_t$ are associated with the drift term. The drift term is a d-dimensional vector, $\vec{a} : [0, T] \times \Re^d \to \Re^d$ and the diffusion term is a $d \times m$ matrix function such that $\mathbf{B} : [0, T] \times \Re^d \to \Re^{d \times m}$. That is to say that the stochastic differential equation for $\vec{X}$ is given by

$$d\vec{X}_t = \vec{a}(t, \vec{X}_{t-}) \, dt + \mathbf{B}(t, \vec{X}_{t-}) \, d\vec{W}_t + \vec{J}(t) \tag{11}$$

where the finite number of bounded jumps is represented by $\vec{J}(t)$. The continuous part is given by Equation[12]. The manner in which $\vec{J}(t)$ is included in the drift term is discussed below.

$$d\vec{X^c}_t = \vec{a}(t, \vec{X^c}_t)\, dt + \mathbf{B}(t, \vec{X^c}_t)\, d\vec{W}_t \tag{12}$$

In keeping with Section 5 of Dean and Russell[2], we let

$$f(t, \vec{x}) = g(\vec{x})$$

thus removing the explicit dependence of f on t.

$$\begin{aligned} g(\vec{X}_t) &= g(\vec{X}_0) + \sum_{j=1}^{d} \int_0^t g_j(\vec{X}_{s-})\, dX_s^j - \sum_{0<s\le t} \sum_{j=1}^{d} g_j(\vec{X}_{s-})\, \Delta X_s^j \\ &+ \frac{1}{2} \sum_{j=1}^{d} \sum_{k=1}^{d} \int_0^t g_{jk}(\vec{X}_{s-})\, d[X^j, X^k]_s^c \end{aligned} \tag{13}$$

We use the fact that the operation $(X, Y) \to [X, Y]$ is bilinear and symmetric and assume for simplicity that $\mathbf{B}(\cdot, \cdot)$ is diagonal and that $X_0^j = 0$.

Formally substituting Equation[11] into Equation[13],

$$\begin{aligned} g(\vec{X}_t) &= g(0) + \sum_{j=1}^{d} \int_0^t g_j(\vec{X}_{s-}) \left(a^j(s, \vec{X}_{s-})\, ds + \mathbf{B}^{jj}(s, \vec{X}_{s-})\, dW_s^j + J^j(s) \right) \\ &- \sum_{0<s\le t} \sum_{j=1}^{d} g_j(\vec{X}_{s-})\, \Delta X_s^j \\ &+ \frac{1}{2} \sum_{j=1}^{d} \sum_{k=1}^{d} \int_0^t g_{jk}(\vec{X}_{s-})\, d[X^j, X^k]_s^c \end{aligned} \tag{14}$$

Using Equation[12], the term $[X^j, X^k]_s^c$ can be expanded as

$$[X^j, X^k]_s^c = \left[\int a^j\, d\tau + \int \mathbf{B}^{jj}\, dW^j, \int a^k\, d\tau + \int \mathbf{B}^{kk}\, dW^k \right]_s$$

Then, applying the bilinearity of the bracket process,

$$\begin{aligned} [X^j, X^k]_s^c &= \left[\int a^j\, d\tau, \int a^k\, d\tau \right]_s + \left[\int a^j\, d\tau, \int \mathbf{B}^{kk}\, dW^k \right]_s \\ &+ \left[\int \mathbf{B}^{jj}\, dW^j, \int a^k\, d\tau \right]_s + \left[\int \mathbf{B}^{jj}\, dW^j, \int \mathbf{B}^{kk}\, dW^k \right]_s \end{aligned}$$

Theorem 29, page 75 of Protter[5] is applied to write this as

$$\begin{aligned} [X^j, X^k]_s^c &= \int_0^s a^j a^k\, d\left[\tau, \tau\right]_u + \int_0^s a^j \mathbf{B}^{kk}\, d\left[\tau, W^k\right]_u \\ &+ \int_0^s \mathbf{B}^{jj} a^k\, d\left[W^j, \tau\right]_u + \int_0^s \mathbf{B}^{jj} \mathbf{B}^{kk}\, d\left[W^j, W^k\right]_u \end{aligned}$$

From Theorem 26, page 71 of Protter[5], the continuous process $X_t = t$ is a quadratic pure jump process . Therefore, $[X, X]_t^c = [X, X]_t = 0$. And, Theorem 29, Protter[5], if $X_t = t$ and $Y_t = W_t$, then

$$[X,Y]_t = X_0Y_0 + \sum_{0<s\leq t} \Delta X_s \Delta Y_s = 0$$

Hence it is clear that $[\tau,\tau] = [\tau,W] = 0$. Furthermore, for a standard $\Re^d$ Brownian motion we have, Protter[4], Chung and Williams[1], Revus and Yor [6],

$$\left[W^j, W^k\right]_u = \begin{cases} u & \text{if } k = j \\ 0 & \text{if } k \neq j \end{cases} \tag{15}$$

We conclude that

$$\left[X^j, X^k\right]_s^c = \begin{cases} \int_0^s (\mathbf{B}^{jj})^2 \, du & \text{if } k = j \\ 0 & \text{if } k \neq j \end{cases}$$

Therefore, we can say that

$$d\left[X^j, X^j\right]_s^c = \left(\mathbf{B}^{jj}\right)^2 \, ds$$

In the case that $\mathbf{B}$ is a full matrix, the i^{th} component of Equation[12] becomes

$$X^i = \int a^i \, d\tau + \sum_{l=1}^m \int \mathbf{B}^{il} \, dW^l \tag{16}$$

from which it follows from Equation[15] that

$$\begin{aligned} \left[\sum_{l=1}^m \int \mathbf{B}^{jl} \, dW^l, \sum_{n=1}^m \int \mathbf{B}^{kn} \, dW^l\right]_s &= \sum_{l=1}^m \sum_{n=1}^m \left[\int \mathbf{B}^{jl} \, dW^l, \int \mathbf{B}^{kn} \, dW^n\right]_s \\ &= \sum_{l=1}^m \int_0^s \mathbf{B}^{jl}\mathbf{B}^{kn} \, d[W^l, W^l]_u \\ &= \sum_{l=1}^m \int_0^s \mathbf{B}^{jl}\mathbf{B}^{kl} \, du \\ &= \int_0^s \left[\mathbf{B}\mathbf{B}^{\mathsf{T}}\right]_{jk} \, du \end{aligned}$$

So that

$$d\left[X^j, X^k\right]_s^c = \left[\mathbf{B}\mathbf{B}^{\mathsf{T}}\right]_{jk} \, ds \tag{17}$$

Substitute Equation[16] and Equation[17] into Equation[14] to obtain

$$\begin{aligned} g(\vec{X}_t) &= g(0) + \sum_{j=1}^d \int_0^t g_j(\vec{X}_{s-}) \, a^j(s, \vec{X}_{s-}) \, ds + \sum_{j=1}^d \int_0^t g_j(\vec{X}_{s-}) J^j(s) \\ &+ \sum_{j=1}^d \int_0^t g_j(\vec{X}_{s-}) \sum_{l=1}^m \mathbf{B}^{jl}(s, \vec{X}_{s-}) \, dW_s^l \\ &- \sum_{0<s\leq t} \sum_{j=1}^d g_j(\vec{X}_{s-}) \, \Delta X_s^j \\ &+ \frac{1}{2} \sum_{j=1}^d \sum_{k=1}^d \int_0^t g_{jk}(\vec{X}_{s-}) \, \left[\mathbf{B}\mathbf{B}^{\mathsf{T}}\right]_{jk} \, ds \end{aligned} \tag{18}$$

The integrals of the form $\int_0^t g_j(\vec{X}_{s-})\ J^j(t)$ will be discussed below, but we can say, loosely, that if the jumps occur in the integrand, then the integral does not record them. However, if the jumps occur in the integrator, then the integral does record the jumps. See Protter[5], Theorem 13, page 60.

When we apply the expectation operator to Equation[18], the Itô integrals will disappear since their expected values are always zero.

If Equation[18] is to make any sense, then there can be no jumps on the RHS. This means that we have to deal with the term

$$\sum_{0<s\leq t} \sum_{j=1}^{d} g_j(\vec{X}_{s-})\ \Delta X_s^j$$

From the proof of the Itô theorem, Protter[5], it follows that this term represents the jumps in the integrals $\sum_{j=1}^{d} \int_0^t g_j(\vec{X}_{s-})\ dX_s^j$, as shown in Equation[13]. Since this term is subtracted, this means that there are no jumps represented on either side of Equation[13]. We must insure that the integrals on the first line of Equation[18] have the appropriate jumps built in.

To do this, recall that our fundamental assumption regarding the jumps is that there are only a finite number of them and they are bounded. On the segments of time where $\vec{X}_t$ is continuous, let

$$Y_t^j = \int_0^t a^j(s, \vec{X}_s)\ ds \quad \Rightarrow \quad dY_t^j = a^j(t, \vec{X}_t)\ dt$$

According to the assumptions of the problem, $\vec{X}_t$ will experience jumps at the interfaces between computational cells with different permeabilities because of the capillary end effect. In order for the stochastic integrals to record these jumps, the process Y^j has to jump at these times also. Let

$$\hat{Y}_t^j = Y_t^j + \sum_{0<s\leq t} \Delta X_s^j \tag{19}$$

As given in Protter[5], the stochastic integral is defined as the *ucp* limit of sums which is given by the following

Definition: A sequence of processes $(H^n)_{n\geq 1}$ converges to a process H *uniformly on compacts in probability (ucp)* if, for each $t > 0$, $\sup_{0\leq s\leq t} |H_s^n - H_s|$ converges to 0 in probability.

Consider the integral

$$\int_0^t g_j(\vec{X}_{s-})\ d\hat{Y}_s^j$$

Using the Theorem 21, page 64 of Protter[5], the stochastic integral $(g_j\_) \cdot \hat{Y}$ can be expressed as the limit in ucp of the Lebesque-Stieltjes sum $\sum_i g_j(\vec{X}_{T_i^n}) \left(\hat{Y}^{T_{i+1}^n} - \hat{Y}^{T_i^n}\right)$, where $\sigma_n : T_0^n \leq T_1^n \leq \cdots \leq T_{i_n}^n$ is an element of a random partition that *tends to the identity* as defined in Protter[5], page 64.

In the proof of Itô's theorem in Protter[5], the following notation is used:

$$\sum_{i,A} \equiv \sum_i \mathbf{I}_{\{A\cap(T_i^n, T_{i+1}^n]\neq\emptyset\}}$$

In our case, the set A is the set of a finite number of bounded jumps. By this we assume that for almost all ω the sample paths have only a finite number of bounded jumps. With this notation, we can use Equation[19] to write

$$\begin{aligned}\sum_i g_j(\vec{X}_{T_i^n})\left((\hat{Y}^j)^{T_{i+1}^n}-(\hat{Y}^j)^{T_i^n}\right) &= \sum_i g_j(\vec{X}_{T_i^n})\left((Y^j)^{T_{i+1}^n}-(Y^j)^{T_i^n}\right)\\ &+ \sum_{i,A} g_j(\vec{X}_{T_i^n})\left((X^j)^{T_{i+1}^n}-(X^j)^{T_i^n}\right)\end{aligned}$$

The sum on the LHS converges in ucp to $\int_0^t g_j(\vec{X}_{s-})\,d\hat{Y}_s^j$; the first sum on the RHS converges in ucp to $\int_0^t g_j(\vec{X}_{s-})a^j(s,\vec{X}_{s-})\,ds$; the second sum on the RHS converges in ucp to $\sum_{0<s\le t} g_j(\vec{X}_{s-})\Delta X_s^j$, to give

$$\int_0^t g_j(\vec{X}_{s-})\,d\hat{Y}_s^j = \int_0^t g_j(\vec{X}_{s-})a^j(s,\vec{X}_{s-})\,ds + \sum_{0<s\le t} g_j(\vec{X}_{s-})\Delta X_s^j$$

Equation[18] can then be written as

$$\begin{aligned}g(\vec{X}_t) &= g(0)+\sum_{j=1}^d\int_0^t g_j(\vec{X}_{s-})\,a^j(s,\vec{X}_{s-})\,ds\\ &+ \sum_{j=1}^d\int_0^t g_j(\vec{X}_{s-})\sum_{l=1}^m \mathbf{B}^{jl}(s,\vec{X}_{s-})\,dW_s^l\\ &+ \frac{1}{2}\sum_{j=1}^d\sum_{k=1}^d\int_0^t g_{jk}(\vec{X}_{s-})\,\left[\mathbf{B}\mathbf{B}^{\mathsf{T}}\right]_{jk}\,ds\end{aligned} \tag{20}$$

In vector notation this becomes

$$\begin{aligned}g(\vec{X}_t) &= g(0)+\int_0^t \nabla g(\vec{X}_{s-})\cdot\vec{a}(s,\vec{X}_{s-})\,ds+\int_0^t \nabla g(\vec{X}_{s-})\cdot\mathbf{B}\vec{W}_s\\ &+ \frac{1}{2}\sum_{j=1}^d\sum_{k=1}^d\int_0^t g_{jk}(\vec{X}_{s-})\,\left[\mathbf{B}\mathbf{B}^{\mathsf{T}}\right]_{jk}\,ds\end{aligned} \tag{21}$$

Next, taking differentials followed by taking expectations and using the property of the Itô integral that its expected value is zero,

$$\frac{d}{dt}\mathbf{E}\left[g(\vec{X}_t)\right] = \mathbf{E}\left[\nabla g(\vec{X}_{t-})\cdot\vec{a}(t,\vec{X}_{t-})+\frac{1}{2}\sum_{j=1}^d\sum_{k=1}^d g_{jk}(\vec{X}_{t-})\,\left[\mathbf{B}\mathbf{B}^{\mathsf{T}}\right]_{jk}\right] \tag{22}$$

Since we have gone to the trouble of removing the jumps, Equation[22] is actually an expression for $\vec{X}^c$, see Equation[12]. In order to get the jumps back into this equation, we can add the expected value of the jumps to the RHS of Equation[22].

$$\begin{aligned}\frac{d}{dt}\mathbf{E}\left[g(\vec{X}_t)\right] &= \mathbf{E}\left[\nabla g(\vec{X}_{t-})\cdot\vec{a}(t,\vec{X}_{t-})+\frac{1}{2}\sum_{j=1}^d\sum_{k=1}^d g_{jk}(\vec{X}_{t-})\,\left[\mathbf{B}\mathbf{B}^{\mathsf{T}}\right]_{jk}\right]\\ &+ \mathbf{E}\left[\sum_{0<s\le t}\nabla g(\vec{X}_{s-})\cdot\Delta\vec{X}_s\right]\end{aligned} \tag{23}$$

The first expected value on the RHS of Equation[23] is the expected value in the interior of a computational cell where the permeability is uniform. The second expected value on the RHS is the expected value at the surface interface between two computational cells of different permeability. We represent this boundary interface as $\partial\Omega$. This expected value can be thought of as being based on one of the marginal densities of $p(\vec{x},t)$.

Let $p(\vec{x},t) \equiv p(\vec{x},t;\vec{x}_0,t_0)$ be the conditional probability density of a particle starting at $\vec{x}_0$ at time t_0. Then,

$$\begin{aligned}
\frac{d}{dt}\mathbf{E}\left[g(\vec{X}_t)\right] &= \frac{d}{dt}\int g(\vec{x})p(\vec{x},t)\,d\vec{x} = \int g(\vec{x})\frac{\partial p}{\partial t}(\vec{x},t)\,d\vec{x} \\
&= \int \nabla g(\vec{x})\cdot\vec{a}(t,\vec{x})p(\vec{x},t)d\vec{x} + \frac{1}{2}\sum_{j=1}^{d}\sum_{k=1}^{d}\int g_{jk}(\vec{x})\ \left[\mathbf{B}\mathbf{B}^{\mathsf{T}}\right]_{jk} p(\vec{x},t)\,d\vec{x} \\
&\quad + \sum_{0<s\leq t}\int \nabla g(\vec{x})\cdot\Delta\vec{x}\,p(\vec{x},t)\,d\vec{x} \qquad (24)
\end{aligned}$$

Next, we want to integrate by parts in order to move the derivatives off $g(\vec{x})$ and onto the other terms in Equation[24]. In doing this we will ignore the surface terms associated with the second line in Equation[24] because it represents behavior in the interior of a computational cell whereas the third line represents behavior on the boundary of the computational cell. In the equations that follow, the term $\Delta\vec{x}$ is best interpreted as the magnitude of the jump times a Heaviside step function which jumps at the interface between two computational cells of different permeabilities. In this way, spatial derivatives of it will be δ-distributions.

$$\begin{aligned}
\int\Bigg[&\frac{\partial p}{\partial t}(\vec{x},t) + \nabla\cdot(\vec{a}(t,\vec{x})p(\vec{x},t)) \\
&- \frac{1}{2}\sum_{j=1}^{d}\sum_{k=1}^{d}\partial_j\partial_k\left(\left[\mathbf{B}\mathbf{B}^{\mathsf{T}}\right]_{jk}p(\vec{x},t)\right) \\
&- \sum_{0<s\leq t}\nabla\cdot(\Delta\vec{x}\,p(\vec{x},t))\Bigg]\,g(\vec{x})\,d\vec{x} = 0 \qquad (25)
\end{aligned}$$

Since $g(\vec{x})$ in Equation[25] is essentially arbitrary, we can write

$$\begin{aligned}
\frac{\partial p}{\partial t}(\vec{x},t) + \nabla\cdot(\vec{a}(t,\vec{x})p(\vec{x},t)) &- \frac{1}{2}\sum_{j=1}^{d}\sum_{k=1}^{d}\partial_j\partial_k\left(\left[\mathbf{B}\mathbf{B}^{\mathsf{T}}\right]_{jk}p(\vec{x},t)\right) \\
&- \sum_{0<s\leq t}\nabla\cdot(\Delta\vec{x}\,p(\vec{x},t)) = 0 \qquad (26)
\end{aligned}$$

To simplify notation, let $\mathbf{C}(t,\vec{x}) = \frac{1}{2}\mathbf{B}(t,\vec{x})\mathbf{B}^{\mathsf{T}}(t,\vec{x})$ so that

$$\begin{aligned}
\frac{\partial p}{\partial t}(\vec{x},t) + \nabla\cdot(\vec{a}(t,\vec{x})p(\vec{x},t)) &- \sum_{j=1}^{d}\sum_{k=1}^{d}\partial_j\partial_k\left(\mathbf{C}_{jk}(t,\vec{x})p(\vec{x},t)\right) \\
&- \sum_{0<s\leq t}\nabla\cdot(\Delta\vec{x}\,p(\vec{x},t)) = 0 \qquad (27)
\end{aligned}$$

Expanding the third term on the left hand side, (summations implied)

$$\partial x_i \partial x_j \left(\mathbf{C}_{ij}(t,\vec{x})p(\vec{x},t)\right) = \overbrace{\left(\nabla \cdot \left(\nabla^{\mathsf{T}}\mathbf{C}^{\mathsf{T}}\right)\right)}^{\partial x_i \partial x_j \mathbf{C}_{ij}(t,\vec{x})} p(\vec{x},t) + \overbrace{\left(\nabla^{\mathsf{T}}\mathbf{C}^{\mathsf{T}}\right) \cdot \nabla p(\vec{x},t)}^{(\partial x_j \mathbf{C}_{ij}(t,\vec{x}))\partial x_i p(\vec{x},t)} + \overbrace{\nabla \cdot \mathbf{C}\nabla p(\vec{x},t)}^{\partial x_i(\mathbf{C}_{ij}(t,\vec{x})\partial x_j p(\vec{x},t))} \tag{28}$$

Expansion of the fourth term on the LHS of Equation[27] yields

$$\sum_{0<s\leq t} \left(\nabla \cdot \Delta\vec{x}\, p(\vec{x},t) + \Delta\vec{x} \cdot \nabla p(\vec{x},t)\right) \tag{29}$$

Next, combine the first term in Equation[29] with the first term on the RHS of Equation[28] and combine the second term in Equation[29] with the second term in Equation[28] to get

$$\nabla \cdot \left(\nabla^{\mathsf{T}}\mathbf{C}^{\mathsf{T}} + \sum_{0<s\leq t} \Delta\vec{x}\right) p(\vec{x},t) + \left(\nabla^{\mathsf{T}}\mathbf{C}^{\mathsf{T}} + \sum_{0<s\leq t} \Delta\vec{x}\right) \cdot \nabla p(\vec{x},t) \tag{30}$$

Applying the product rule for the divergence to Equation[30] this can be written as

$$\nabla \cdot \left[\left(\nabla^{\mathsf{T}}\mathbf{C}^{\mathsf{T}} + \sum_{0<s\leq t} \Delta\vec{x}\right) p(\vec{x},t)\right] \tag{31}$$

On substitution of Equation[31] into Equation[27] and using the linearity of the divergence operator,

$$\frac{\partial p(\vec{x},t)}{\partial t} + \nabla \cdot \left[\left(\vec{a}(t,\vec{x}) - \nabla^{\mathsf{T}}\mathbf{C}^{\mathsf{T}}(t,\vec{x}) - \sum_{0<s\leq t} \Delta\vec{x}\right) p(\vec{x},t)\right] - \nabla \cdot \mathbf{C}(t,\vec{x})\nabla p(\vec{x},t) = 0 \tag{32}$$

In Section 4 of Dean and Russell[2] is Equation[12] which is a PDE for $p(\vec{x},t)$ based on Darcy's law and the continuity equation. In order for Equation[32] to match Dean and Russell[2], Equation[12], we must have (for the α-phase)

$$\vec{a}(t,\vec{x}) = \frac{1}{\theta_\alpha(t,\vec{x})}\mathbf{K}_\alpha\left(\theta_\alpha(t,\vec{x})\right)\vec{z} + \nabla^{\mathsf{T}}\mathbf{C}^{\mathsf{T}}(t,\vec{x}) + \sum_{0<s\leq t} \Delta\vec{x}$$

and

$$\mathbf{C}(t,\vec{x}) = \frac{1}{2}\mathbf{B}(t,\vec{x})\mathbf{B}^{\mathsf{T}}(t,\vec{x}) = \mathbf{D}\left(\theta_\alpha(t,\vec{x})\right)$$

Since we originally subtracted out of $\vec{a}(t,\vec{x})$ the jumps as $\vec{J}(t)$, they get added back in to the drift term at this point. Using these coefficients in the SDE gives

$$d\vec{X}_t = \left[\frac{1}{\theta_\alpha(t,\vec{X}_t)}\mathbf{K}_\alpha\left(\theta_\alpha(t,\vec{X}_t)\right)\vec{z} + \nabla^{\mathsf{T}}\mathbf{D}^{\mathsf{T}}(t,\vec{X}_t) + \sum_{0<s\leq t} \Delta\vec{X}_s\right] dt + \mathbf{B}(t,\vec{X}_t)\, d\vec{W}_t \tag{33}$$

Suppose that the particle is moving from a computational cell containing a coarse sand, C_i to a computational cell containing a fine sand, C_j. $B = C_i \cap C_j$ is the common boundary between the

two computational cells. In this example, the flow is assumed to be in the negative z-direction, as shown in Figure 2.

The capillary diffusivity can change suddenly at the boundary B between the computational cells C_i and C_j. This sudden change can cause pooling along the boundary B.

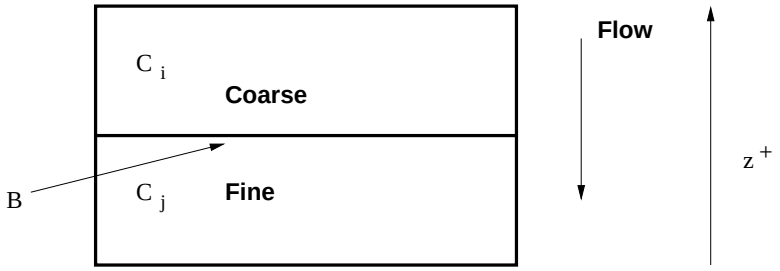

Figure 2: Coarse/Fine Computational Interface

In Dean and Russell[2], Appendix A, the effect of this jump is quantified using Green's formula. We want to relate that result to the jumps $\Delta\vec{X}_s$.

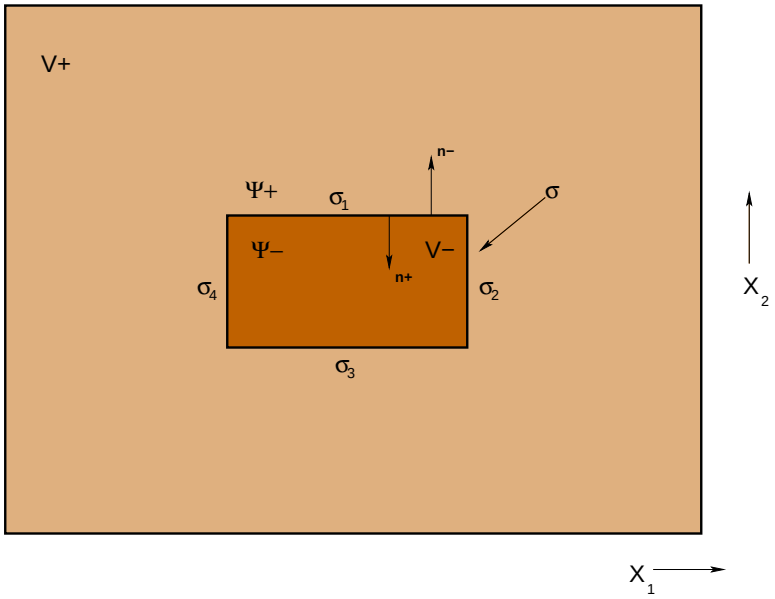

Figure 3: Sands With Discontinuity

In Figure 3, the domain of the experimental tank is divided into two subdomains $V+$ and $V-$. Subdomain $V+$ consists of a high permeability sand and $V-$ consists of a low permeability sand. The boundary of the low permeability sand is marked by $\sigma = \sigma_1 \cup \sigma_2 \cup \sigma_3 \cup \sigma_4$. $\Psi^+ = \lim_{\vec{x}\to\sigma+} \Psi$ and $\Psi^- = \lim_{\vec{x}\to\sigma-} \Psi$, where Ψ represents a component of capillary diffusivity. The quantity $[[\Psi]] = \Psi^+ - \Psi^-$. The vector $\mathbf{n}^+$ is the unit normal vector pointing out of the positive region, $V+$, and $\mathbf{n}^-$ is the unit normal vector pointing out of the negative region, $V-$.

The diffusivity is given by

$$\mathbf{D} = \bar{\lambda}\mathbf{k}\frac{dp_c}{d\theta_n}$$

and from the definition of $\Delta\vec{X}_t$, see page 2, if s is a jump time, then

$$\Delta\vec{X}_s = \vec{X}_s - \vec{X}_{s-} = \vec{X}_s - \lim_{t\to s,\ t<s} \vec{X}_t$$

Since $\vec{X}_t$ is càdlàg and the sample is moving from V^+ to V^- over time, it follows that $\vec{X}_s \in V^-$, the limit $\vec{X}_{s-}$ is based on $\vec{X}_t \in V^+$ and

$$\begin{aligned} \Delta\vec{X}_s &= \left(\mathbf{D}^- - \mathbf{D}^+\right)\vec{n}^+\,\delta\left(\partial\Omega\right) \\ &= -[[\mathbf{D}]]\vec{n}^+\,\delta\left(\partial\Omega\right) \end{aligned}$$

Equation[33] then becomes

$$\begin{aligned} d\vec{X}_t &= \left[\frac{1}{\theta_\alpha(t,\vec{X}_t)}\mathbf{K}_\alpha\left(\theta_\alpha(t,\vec{X}_t)\right)\vec{z} + \nabla^{\mathsf{T}}\mathbf{D}^{\mathsf{T}}(t,\vec{X}_t) - \sum_{0<s\leq t}[[\mathbf{D}]]\vec{n}^+\,\delta\left(\partial\Omega\right)\right]dt \\ &\quad + \mathbf{B}(t,\vec{X}_t)\,d\vec{W}_t \end{aligned} \tag{34}$$

Equation[34] should be compared with Equation[17] in Dean and Russell[2]. The only difference is that Equation[34] accomodates directly the jumps in a sample path, whereas in the case of Equation[17], additional processing is required to interpret the term $\nabla^{\mathsf{T}}\mathbf{D}^{\mathsf{T}}$ as a distributional derivative, see Dean and Russell[2], Appendix A, Equation[35].

The approach adopted here is more natural. Equation[23] is Equation[22] with the expected effect of the jumps added. The first term on the RHS of Equation[23] derives from a continuous semimartingale. In other words, it describes the expected behavior on the interior of a computational cell where $\vec{X}_t$ is continuous. The second term on the RHS of Equation[23] describes the expected behavior on a boundary between two computational cells of different permeability.

The outcome of the subsequent argument is Equation[34] where the term $\nabla^{\mathsf{T}}\mathbf{D}^{\mathsf{T}}$, if applicable, applies to the interior of a computational cell and the term $\sum_{0<s\leq t}[[\mathbf{D}]]\vec{n}^+\,\delta\left(\partial\Omega\right)$, if applicable, applies to the boundary.

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