Stochastic Differential Equations In Transport
Moment Equations

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ABSTRACT

In previous reports (cf. Dean and Russell[36], Dean[35]), the application of stochastic differential equations to transport in porous media is discussed. The methods described in those reports can be used in a Monte Carlo setting to develop estimates of the statistical moments of the contaminant plumes's probability distribution. A second method of developing this type of statistical information is to derive a system of partial differential equations in which the statistical moments appear as the independent variables to be determined. This report describes the application of the Itô theory to the development of a system of partial differential equations in terms of the first and second moments. As applications of this method, two examples are given. The first application uses the results of the theory to derive a system of moment equations as found in Graham And McLaughlin[50]. For comparison purposes, this system is derived in an *ad hoc* manner in Section 2 using the method of distributed parameters. The second example uses the theoretical moment equations to incorporate the effects of measurement error in a concentration covariance equation.

1 Introduction

Permeability, density and viscosity are related through hydraulic conductivity. So, both soil properties and fluid properties are represented in hydraulic conductivity. Furthermore, hydraulic conductivity determines the velocity field of the water in the aquifer, and if a solute is introduced into the aquifer, the path a solute particle takes through the aquifer is determined by two components. First, the path has a component that is due to molecular diffusion and, secondly, a component that is due to the mechanical mixing that results from the convective transport. This means that the developing plume is dispersing about a path that is changing due to the influence of the convective transport determined by the large-scale heterogeneities of the aquifer's domain. In Dean[35], Dean and Russell[36] one method of determining the dispersion used in the transport equation is discussed, and implemented to estimate the expected value of the concentration of a tracer injected into a test tank. The entire approach is based on stochastic descriptions of the hydraulic conductivities of the 5 different types of sands with which the tank is packed. As explained in Dean and Russell[36], Dean[35], the domain is subdivided into rectangular grid blocks, each of which is assigned its own average velocity and dispersion coefficient computed according to the methodology explained therein. This approach provides the domain of the aquifer with a velocity field that mimicks large-scale changes in the permeabilities of the different sections. However, only the expected value of the concentration is predicted. What is needed in addition to this is a system that will provide information on higher order moments. In general, the more moments that are known, the better the probability density can be described. It would be desirable to at least know something about the second moments.

The purpose of this report is to analyze two methods of providing information on higher moments. In the first method, the second moments are derived from the transport equation by a method of distributed parameters. The second method involves the theory of stochastic differential equations. For the second method, an approach using the Itô calculus, specifically Itô's lemma, is used.

2 Moments Derived From Distributed Parameters

The first method is based on the work of Graham And McLaughlin[50] who derive *unconditional* ensemble moments, ie, moments that do not depend on concentration observations. Starting from the transport equation,

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\vec{V}) - \nabla \cdot [\mathbf{D}\nabla c] = 0 \tag{1}$$

and letting

$$c = \mathbf{E}[c] + c' \quad \vec{V} = \mathbf{E}[\vec{V}] + \vec{V'} \quad \mathbf{E}[c'] = 0 \quad \mathbf{E}[\vec{V'}] = 0 \tag{2}$$

we get by substituting Equation[2] into Equation[1]

$$\begin{aligned} \frac{\partial \mathbf{E}[c]}{\partial t} + \frac{\partial c'}{\partial t} &+ \nabla \cdot \left[\mathbf{E}[c]\mathbf{E}[\vec{V}] + \mathbf{E}[c]\vec{V'} + \mathbf{E}[\vec{V}]c' + c'\vec{V'}\right] \\ &- \nabla \cdot [\mathbf{D}\nabla \mathbf{E}[c] + \mathbf{D}\nabla c'] = 0 \end{aligned} \tag{3}$$

and by taking expectations and using $\mathbf{E}[c'] = \mathbf{E}[\vec{V'}] = 0$, we get the *mean concentration equation*

$$\frac{\partial \mathbf{E}[c]}{\partial t} + \nabla \cdot \left(\mathbf{E}[c]\mathbf{E}[\vec{V}]\right) - \nabla \cdot (\mathbf{D}\nabla \mathbf{E}[c]) + \nabla \cdot \mathbf{E}[c'\vec{V'}] = 0 \tag{4}$$

Subtracting Equation[4] from Equation[3] we get an equation that involves the perturbations of the concentration and the velocity field

$$\begin{aligned} \frac{\partial c'}{\partial t} + \nabla \cdot \mathbf{E}[c]\vec{V'} &+ \nabla \cdot \mathbf{E}[\vec{V}]c' + \nabla \cdot (c'\vec{V'}) \\ &- \nabla \cdot \mathbf{D}\nabla c' - \nabla \cdot \mathbf{E}[c'\vec{V'}] = 0 \end{aligned} \tag{5}$$

Multiply Equation[5] by the perturbed velocity vector at a point $\vec{x'}$ different from $\vec{x}$. Since the velocity perturbation depends only on the spatial variable and $\vec{x'}$ is different from $\vec{x}$ and the derivatives are taken at $\vec{x}$, it follows that

$$\begin{aligned} \frac{\partial (c'\vec{V'}(\vec{x'}))}{\partial t} &+ \left(\nabla_{\vec{x}} \cdot \mathbf{E}[c]\vec{V'}(\vec{x})\right) \vec{V'}(\vec{x'}) + \nabla_{\vec{x}} \cdot \mathbf{E}[\vec{V}]c'\vec{V'}(\vec{x'}) \\ &+ \nabla_{\vec{x}} \cdot \left(c'\vec{V'}(\vec{x})\right) \vec{V'}(\vec{x'}) - \nabla_{\vec{x}} \cdot \mathbf{D}\nabla_{\vec{x}} c'\vec{V'}(\vec{x'}) \\ &- \nabla_{\vec{x}} \cdot \mathbf{E}[c'\vec{V'}(\vec{x})]\vec{V'}(\vec{x'}) = 0 \end{aligned}$$

The i^{th} component of this equation is written

$$\begin{aligned} \frac{\partial (c'V_i'(\vec{x'}))}{\partial t} &+ \left(\frac{\partial}{\partial x_j}(\mathbf{E}[c]V_j'(\vec{x})\right) V_i'(\vec{x'}) \\ &+ \frac{\partial}{\partial x_j}\left(\mathbf{E}[V_j]c'\right) V_i'(\vec{x'}) + \frac{\partial}{\partial x_j}\left(c'V_j'(\vec{x})\right) V_i'(\vec{x'}) \\ &- \frac{\partial}{\partial x_j}\left(D_{jk}\frac{\partial}{\partial x_k}(c')\right) V_i'(\vec{x'}) - \frac{\partial}{\partial x_j}\left(\mathbf{E}[c'V_j'(\vec{x})]\right) V_i'(\vec{x'}) = 0 \end{aligned}$$

Since the components V_i' are evaluated at $\vec{x'}$, they are constants with respect to the $\frac{\partial}{\partial x_j}$ operator, and so we can write

$$\begin{aligned} \frac{\partial (c'V_i'(\vec{x'}))}{\partial t} &+ \frac{\partial}{\partial x_j}\left(\mathbf{E}[c]V_j'(\vec{x})V_i'(\vec{x'})\right) \\ &+ \frac{\partial}{\partial x_j}\left(\mathbf{E}[V_j]c'V_i'(\vec{x'})\right) + \frac{\partial}{\partial x_j}\left(c'V_j'(\vec{x})V_i'(\vec{x'})\right) \\ &- \frac{\partial}{\partial x_j}\left(D_{jk}\frac{\partial}{\partial x_k}(c'V_i'(\vec{x'}))\right) - \frac{\partial}{\partial x_j}\left(\mathbf{E}[c'V_j'(\vec{x})]V_i'(\vec{x'})\right) = 0 \end{aligned} \tag{6}$$

Define

$$
\begin{aligned}
C_{V_i c}(\vec{x'}, \vec{x}, t) &= \mathbf{E}[V_i'(\vec{x'}) c(\vec{x}, t)] \\
C_{V_i V_j}(\vec{x'}, \vec{x}) &= \mathbf{E}[V_i'(\vec{x'}) V_j'(\vec{x})] \\
C_{cV_i V_j}(\vec{x'}, \vec{x}, t) &= \mathbf{E}[c'(\vec{x}, t) V_i'(\vec{x'}) V_j'(\vec{x})] \\
C_{cc}(\vec{x'}, \vec{x}, t) &= \mathbf{E}[c'(\vec{x'}, t) c'(\vec{x}, t)]
\end{aligned}
$$

Taking expectations of Equation[6] yields the *velocity-concentration covariance* equation.

$$
\begin{aligned}
\frac{\partial}{\partial t} C_{cV_i}(\vec{x'}, \vec{x}, t) &+ \frac{\partial}{\partial x_j} \mathbf{E}[c] C_{V_i V_j}(\vec{x'}, \vec{x}) \\
&+ \frac{\partial}{\partial x_j} \mathbf{E}[V_j] C_{cV_i}(\vec{x'}, \vec{x}, t) \\
&+ \frac{\partial}{\partial x_j} \mathbf{E}[c'(\vec{x}, t) V_j'(\vec{x}) V_i'(\vec{x'})] \\
&- \frac{\partial}{\partial x_j} \left(D_{jk} \frac{\partial}{\partial x_k} C_{cV_i}(\vec{x'}, \vec{x}, t) \right) = 0
\end{aligned}
\tag{7}
$$

Note: The last term in Equation[6] vanishes because $\mathbf{E}[V_i'(\vec{x'})] = 0$.

Taking Equation[5] and multiplying by $c'(\vec{x'}, t)$ where $\vec{x'} \neq \vec{x}$ and using the assumption that $\mathbf{E}[c'(\vec{x'}, t)] = 0$ and the covariance definitions we get

$$
\begin{aligned}
\mathbf{E}\left[\frac{\partial}{\partial t}(c'(\vec{x}, t)) c'(\vec{x'}, t)\right] &+ \frac{\partial}{\partial x_j} \mathbf{E}[c(\vec{x}, t)] C_{V_j c}(\vec{x'}, \vec{x}, t) \\
&+ \frac{\partial}{\partial x_j} \mathbf{E}[V_j(\vec{x})] C_{cc}(\vec{x'}, \vec{x}, t) \\
&+ \frac{\partial}{\partial x_j} \mathbf{E}[c'(\vec{x}, t) c'(\vec{x'}, t) V_j'(\vec{x})] \\
&- \frac{\partial}{\partial x_j} \left[D_{jk} \frac{\partial}{\partial x_k} C_{cc}(\vec{x'}, \vec{x}, t) \right] = 0
\end{aligned}
\tag{8}
$$

Interchanging the roles of $\vec{x'}$ and $\vec{x}$ we get

$$
\begin{aligned}
\mathbf{E}\left[\frac{\partial}{\partial t}(c'(\vec{x'}, t)) c'(\vec{x}, t)\right] &+ \frac{\partial}{\partial x_j'} \mathbf{E}[c(\vec{x'}, t)] C_{V_j c}(\vec{x}, \vec{x'}, t) \\
&+ \frac{\partial}{\partial x_j'} \mathbf{E}[V_j(\vec{x'})] C_{cc}(\vec{x}, \vec{x'}, t) \\
&+ \frac{\partial}{\partial x_j'} \mathbf{E}[c'(\vec{x'}, t) c'(\vec{x}, t) V_j'(\vec{x'})] \\
&- \frac{\partial}{\partial x_j'} \left[D_{jk} \frac{\partial}{\partial x_k'} C_{cc}(\vec{x}, \vec{x'}, t) \right] = 0
\end{aligned}
\tag{9}
$$

Adding Equations [8] and [9] and using the product rule of differentiation

$$
\begin{aligned}
\frac{\partial}{\partial t} C_{cc}(\vec{x'}, \vec{x}, t) &= \frac{\partial}{\partial t} \mathbf{E}[c'(\vec{x'}, t) c'(\vec{x}, t)] \\
&= \mathbf{E}\left[\frac{\partial}{\partial t}(c'(\vec{x'}, t)) c'(\vec{x}, t)\right] + \mathbf{E}\left[\frac{\partial}{\partial t}(c'(\vec{x}, t)) c'(\vec{x'}, t)\right]
\end{aligned}
$$

the following equation for the *concentration covariance* is obtained

$$
\begin{aligned}
\frac{\partial}{\partial t}C_{cc}(\vec{x'},\vec{x},t) &+ \frac{\partial}{\partial x_j}\mathbf{E}[V_j(\vec{x})]C_{cc}(\vec{x'},\vec{x},t) \\
&+ \frac{\partial}{\partial x'_j}\mathbf{E}[V_j(\vec{x'})]C_{cc}(\vec{x},\vec{x'},t) - \frac{\partial}{\partial x_j}\left[D_{jk}\frac{\partial}{\partial x_k}C_{cc}(\vec{x'},\vec{x},t)\right] \\
&- \frac{\partial}{\partial x'_j}\left[D_{jk}\frac{\partial}{\partial x'_k}C_{cc}(\vec{x},\vec{x'},t)\right] + \frac{\partial}{\partial x_j}\mathbf{E}[c(\vec{x},t)]C_{V_j c}(\vec{x'},\vec{x},t) \\
&+ \frac{\partial}{\partial x'_j}\mathbf{E}[c(\vec{x'},t)]C_{V_j c}(\vec{x},\vec{x'},t) + \frac{\partial}{\partial x_j}\mathbf{E}[c'(\vec{x},t)c'(\vec{x'},t)V'_j(\vec{x})] \\
&+ \frac{\partial}{\partial x'_j}\mathbf{E}[c'(\vec{x'},t)c'(\vec{x},t)V'_j(\vec{x'})] = 0 \qquad (10)
\end{aligned}
$$

The *mean concentration equation* can be written using the covariance notation as

$$
\begin{aligned}
\frac{\partial \mathbf{E}[c]}{\partial t} + \sum_{i=1}^{n}\frac{\partial}{\partial x_i}(\mathbf{E}[c]\mathbf{E}[V_i]) &- \sum_{i=1}^{n}\frac{\partial}{\partial x_i}\left[\sum_{j=1}^{n}D_{ij}\frac{\partial}{\partial x_j}\mathbf{E}[c]\right] \\
&+ \sum_{i=1}^{n}\frac{\partial}{\partial x_i}C_{cV_i} = 0
\end{aligned}
$$

This equation has the form of a transport equation with a forcing term that involves the concentration-velocity covariance.

The *velocity-concentration equation*[7] has the form of a transport equation that involves a forcing term that consists of one term that contains the product of the mean concentration and the velocity covariances and one term that involves the expected value of the product of the perturbation of the concentration and velocities. The mean concentration equation and the velocity-concentration covariance are coupled through the $\mathbf{E}[c]$ variable and the C_{cV_i} variable.

The *concentration-covariance equation*[10] also has the form of a transport equation with a forcing term consisting of the last four terms in Equation[10]. The coupling to the other two equations is through the terms $\mathbf{E}[c]$ and C_{cV_i}.

In order to solve this system, the mean velocities and the velocity covariances are required as inputs. The terms, then, that have to be dealt with to form a closed system are

$$
\begin{aligned}
&\tfrac{\partial}{\partial x_j}\mathbf{E}[c'(\vec{x},t)V'_j(\vec{x})V'_i(\vec{x'})] \\
&\tfrac{\partial}{\partial x_j}\mathbf{E}[c'(\vec{x},t)c'(\vec{x'},t)V'_j(\vec{x})] \qquad (11) \\
&\tfrac{\partial}{\partial x_j}\mathbf{E}[c'(\vec{x'},t)c'(\vec{x},t)V'_j(\vec{x'})]
\end{aligned}
$$

These terms are considered to be small, and therefore neglected. To say that these terms can be considered to be small and therefore can be neglected does not seem convincing. By saying that the perturbations are small would certainly imply that the expectations of the products of the perturbations are small, but these terms involve the spatial derivatives of the perturbations and there is no reason to believe that they are small.

These terms can be eliminated if the assumption is made that they come from a multivariate Gaussian distribution. The multivariate Gaussian probability density function for n dependent random variables is given by

$$f(z_1, z_2, \cdots, z_n) = \frac{|\mathbf{V}|^{-\frac{1}{2}}}{(2\pi)^{\frac{n}{2}}} \exp\left\{ -\frac{1}{2}(\vec{z} - \vec{\mu})^\dagger (\mathbf{V}^{-1})(\vec{z} - \vec{\mu}) \right\}$$

where

$$\vec{z} = (z_1, z_2, \cdots, z_n)\dagger$$

$$\vec{\mu} = (\mathbf{E}[z_1], \mathbf{E}[z_2], \cdots, \mathbf{E}[z_n])\dagger$$

$$\mathbf{V} = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1n} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2n} \\ & & \vdots & \\ \sigma_{n1} & \sigma_{n2} & \cdots & \sigma_N^2 \end{pmatrix}$$

So that $\mathbf{V}$ is the variance-covariance matrix.

The multivariate characteristic function is given by, Springer[98], page 75,

$$\phi(\zeta_1, \zeta_2, \cdots, \zeta_n) = \exp\left(-\frac{1}{2}\vec{\zeta}^\dagger \mathbf{V}\vec{\zeta}\right) \exp\left(i\vec{\zeta}^\dagger \vec{\mu}\right)$$

Applying this theory to our problem, consider the trivariate case where

$$\vec{z} = (c'(\vec{x}, t), c'(\vec{x'}, t), V_j'(\vec{x}))^\dagger$$

Since the variations are assumed to have zero means, it follows that

$$\vec{\mu} = 0$$

And, the trivariate characteristic function has the form

$$\phi(\zeta_1, \zeta_2, \zeta_3) = \exp\left(-\frac{1}{2}\vec{\zeta}^\dagger \mathbf{V}\vec{\zeta}\right)$$

The expression $\vec{\zeta}^\dagger \mathbf{V}\vec{\zeta}$ is a quadratic form, and when expanded is equal to

$$\vec{\zeta}^\dagger \mathbf{V}\vec{\zeta} = (\zeta_1, \zeta_2, \zeta_3) \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_2^2 & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \end{bmatrix} = \sum_{i=1}^{3}\sum_{j=1}^{3} \sigma_{ij}\zeta_i\zeta_j$$

So, the trivariate characteristic function is given by

$$\phi(\zeta_1, \zeta_2, \zeta_3) = \exp\left(-\frac{1}{2}\sum_{i=1}^{3}\sum_{j=1}^{3} \sigma_{ij}\zeta_i\zeta_j\right)$$

The reason for introducing the multivariate characteristic function is that moments can be generated from it by taking derivatives. In particular,

$$\mathbf{E}[z_1 z_2 z_3] = \left[\frac{1}{i^3}\frac{\partial^3 \phi(\zeta_1, \zeta_2, \zeta_3)}{\partial\zeta_1 \partial\zeta_2 \partial\zeta_3}\right]_{\zeta_1=\zeta_2=\zeta_3=0}$$

On taking the partial derivatives and using the condition that $\zeta_1 = \zeta_2 = \zeta_3 = 0$, it follows that

$$\mathbf{E}[z_1 z_2 z_3] = 0$$

So, with the assumption of a joint Gaussian distribution the terms in Equation[11] can be removed.

3 An Itô Calculus Approach

3.1 System Definition

A solution is sought for the following system:

$$\begin{aligned}\frac{\partial u}{\partial t} + A(x,t,\omega)u &= g(x,t,\omega) \qquad (x,t,\omega) \in G \times [0,t] \times \Omega \\ Q(x,t,\omega) &= J(\omega) \qquad (x,t,\omega) \in \partial G \times [0,T] \times \Omega \\ u(x,0,\omega) &= u_0(x,\omega) \qquad (x,\omega) \in G \times \Omega\end{aligned} \tag{12}$$

where $g \in L_2(\Omega, \mathcal{B}, P)$ the space of second order random functions.

$G \subset \Re^n$ is an open domain with a Lipshitz continuous boundary, ∂G, and $t \in (0, \infty)$.

The operator A is defined as

$$Au = \sum_{|k|,|l| \leq m} (-1)^{|k|} D^k (p_{kl}(x,t,\omega) D^l u)$$

The operator D represents weak differentiation and the solution $u \in L^2(0,T;V)$, where

$$L^2(0,T;V) = \left\{ f : [0,T] \to V \quad : \quad \int_0^t \|f\|_V^2 dt < \infty \right\}$$

The Hilbert space V represents an m^{th} order Sobolev space of $L^2(\Omega)$-valued random functions on the set G. The space V will be more completely specified in the sub-section entitled **Existence Theory**.

3.2 Types Of Problems

The following is a list of the different types of problems that can potentially be handled using the stochastic evolution equation formulation:

- The random initial value problem; u_0 is random
- The random boundary value problem; J is random
- The random forcing problem; g is random
- The random operator problem; A or Q is random
- The random geometry problem; G is random
- Combinations of the above

In this report, the groundwater transport problem will be treated first as a random operator problem, ie, the operator A will be allowed to have a random component. Secondly, the groundwater transport problem will be treated as a random forcing term problem, ie, g is allowed to be random. The interest here is in techniques for solving the stochastic evolution equations and in determining their first and second moment equations.

First, the problem of existence of solutions has to be addressed. It is necessary to be able to state conditions under which solutions will exist, and be able to specify the spaces that will contain the solutions.

3.3 Existence Theory

The existence theory in this section is compiled from Becus[13], Sawaragi, Soeda, Omatu[90], Serrano, Unny, Lennox[95] and Oden and Reddy[76].

Let $(\Omega, \mathcal{B}, P)$ be a complete probability space and define

$$L_2(\Omega) = L_2(\Omega, \mathcal{B}, P)$$

to be the space of second order random functions on Ω. A probability space is complete if the measure P is complete, *i.e.*, if any subset of a set, $B \in \mathcal{B}$, with $P(B) = 0$, also belongs to $\mathcal{B}$. The space $L_2(\Omega)$ is a Hilbert space with inner product

$$(f, g)_\Omega = \int_\Omega fg dP = \mathbf{E}[fg]$$

Next the following set M is defined

$$M = \{f : G \to L_2(\Omega)\}$$

to be the set of second order random functions on $G \subset \Re^n$.

Using the set M, the following spaces are defined:

$$H = L_2[G; L_2(\Omega)] = \{f \in M : \|f\|_\Omega \in L^2(G)\}$$

where $L^2(G)$ are the square-integrable functions on G.

H is a Hilbert space with inner product

$$\begin{aligned}(f, g)_H &= \int_G (f, g)_\Omega dG = \int_G E[fg] dG \\ &= \int_G \int_\Omega fg dP dG\end{aligned}$$

And, for $m \geq 0$,

$$H^m = H^m(G; L_2(\Omega)) = \{f \in M : D^\alpha f \in H, |\alpha| \leq m\}$$

H^m is a Hilbert space with inner product

$$(f, g)_{H^m} = \sum_{|\alpha| \leq m} (D^\alpha f, D^\alpha g)_H$$

Hence, H^m is the m^{th} order Sobolev space of $L_2(\Omega)$-valued functions on G. Let V be a real separable Hilbert space such that

$$\overline{V} = H$$

and the injection

$$i : V \to H$$

is continuous. It then follows that the following diagram can be established

$$\begin{array}{cccc} & V & \xrightarrow{i} & H & \\ Z_V & \downarrow & & \downarrow & Z_H \\ & V' & \xleftarrow{i'} & H' & \end{array}$$

where the mappings Z_V and Z_H are the Riesz maps between the Hilbert spaces V and its dual V' and between H and its dual H', respectively.

And, by identifying H with its dual, H', it can be shown that

$$V \subset H = H' \subset V'$$

and that H' is densely embedded in V'. Using the Hahn-Banach theorem, the duality pairing on $V' \times V$ can be identified with the unique extension of the duality pairing on $H' \times H$, $< q, u >_H$. And, by the Riesz Representation theorem, $\forall q \in H'$, $\exists\ v_q \in H$ such that

$$< q, u >_H = (v_q, u)_H \qquad \forall u \in H$$

where $(\cdot, \cdot)_H$ is the inner product on H. So, the duality pairing on $V' \times V$ can be identified with the unique extension of the inner product on H.

Given this, the norm on V' can be represented as

$$\begin{aligned} \|\phi\|_{V'} &= \sup_{\substack{u \in V \\ u \neq 0}} \frac{| < \phi, u >_V |}{\|u\|_V} \\ &= \sup_{\substack{u \in V \\ u \neq 0}} \frac{|(v_\phi, u)_H|}{\|u\|_V} \end{aligned}$$

For $0 < T < \infty$, define

$$L^2(0, T; V) = \left\{ f : [0, T] \to V \ \ : \ \ \int_0^T \|f\|_V^2 dt < \infty \right\}$$

And, if $f \in L^2(0, T; V)$, then $D_t f$ is the derivative of f in the sense of V-valued distributions, ie,

$$D_t f \in V'$$

Define

$$W(0, T) = \{ f \in L^2(0, T; V) \ \ : \ \ D_t f \in L^2(0, T; V') \}$$

$W(0,T)$ is a Hilbert space with norm

$$\|f\|_W^2 = \int_0^T \left(\|f\|_V^2 + \|D_t f\|_{V'}^2\right) dt$$

Becus[13] recasts the stochastic evolution equation in its variational form, and letting

$$(A(x,t,\omega)u,v)_H = a(u,v)$$

satisfy

$$|a(u,v)| \leq M\|u\|_V\|v\|_V \qquad \exists\ M > 0$$

and the ellipticity condition that $\exists\lambda$ such that $\forall v \in V$ and for some $\alpha > 0$

$$a(v,v) + \lambda\|v\|_H^2 \geq \alpha\|v\|_V^2$$

for almost all $t \in [0,T]$, proves the following existence theorem.

Theorem: There exists a unique stochastic process $u \in W(0,T)$ as a solution of the system [12]. Also, this solution is continuously dependent on the data, ie, the mapping

$$\{g, u_0\} \rightarrow u$$

is continuous from $L^2(0,T;V') \times H$ to $L^2(0,T;V)$. □

The stochastic partial differential equation found in system [12] can be thought of as a special case of an Itô stochastic partial differential equation of the form

$$du \quad = \quad (-Au + g)\, dt + \Gamma\, dW \tag{13}$$

where W represents a Wiener process. One source of the theoretical details of this type of stochastic partial differential equation in terms of Sobolev spaces is Krylov[63]. In what follows, this type of stochastic partial differential equation will be used to develop the moment equations. Any investigation involving stochastic differential equations such as Equation[13] will involve the Itô calculus, specifically stochastic integration which is introduced next.

3.4 Stochastic Integration

Many discussions of stochastic integrals characterize the stochastic integral in terms of a Wiener or Brownian motion process. Doob[38] generalizes this somewhat to define the stochastic integral in terms of a *martingale*. This term is not very descriptive. In fact, the primary definition in Webster's dictionary is that of a part of a harness for a horse. However, it is also used to describe a system of betting strategies. Of course, probability theory makes this form of the definition more precise. Following Doob[38], Burrill[17] and Jazwinski[56], the major ideas are outlined below. As a matter of convenience the *Radon-Nikodym Theorem* is stated as found in Burrill[17].

Radon-Nikodym Theorem Let the measure μ and the absolutely continuous additive function ϕ be σ-finite. Then there is a finite valued measurable function g such that

$$\phi(E) = \int_E g d\mu$$

for each measurable set E. □

Given a probability space $(\Omega, \mathcal{E}, P)$ and an integrable random variable X on Ω, define the function

$$\phi(E) = \int_E X dP$$

which is an additive function and absolutely continuous relative to P, ($\phi(E) = 0$ if $P(E) = 0$). The set E belongs to a σ-algebra $\mathcal{F}$ contained in $\mathcal{E}$. So, by the Radon-Nikodym Theorem there is an $\mathcal{F}$-measurable function denoted by $\mathbf{E}[X|\mathcal{F}]$ such that

$$\phi(E) = \int_E \mathbf{E}[X|\mathcal{F}] dP = \int_E X dP$$

for each $E \in \mathcal{F}$ and called the *conditional expectation of X given $\mathcal{F}$*. In fact, $\mathbf{E}[X|\mathcal{F}]$ represents an equivalence class of integrable random variables such that any member of the equivalence class is measurable with respect to $\mathcal{F}$ and has the same integral as X over any $E \in \mathcal{F}$.

Next, let

$$T \subset I \cup \{-\infty, +\infty\}$$

where I is the set of integers, and let $\{\mathcal{F}_t : t \in T\}$ be a collection of σ-algebras such that

$$\mathcal{F}_s \subset \mathcal{F}_t \subset \mathcal{E} \quad \text{for} \quad s < t$$

and, finally, let $\{X(t) : t \in T\}$ be a collection on integrable random variables such that $X(t)$ is measurable relative to $\mathcal{F}_t$ for each t. In probability theory, the sets in $\mathcal{F}_t$ are called *events*, and the measurability of $X(t)$ with respect to the σ-algebra $\mathcal{F}_t$ can be interpreted to mean that the values of $X(t)$ are detectable by the events in $\mathcal{F}_t$.

Definition: The collection $\{X(t) : t \in T\}$ is a *martingale* relative to $\{\mathcal{F}_t : t \in T\}$ if

$$X(s) = \mathbf{E}[X(t)|\mathcal{F}_s] \qquad s < t$$

and a *semi-martingale* relative to $\{\mathcal{F}_t : t \in T\}$ if

$$X(s) \leq \mathbf{E}[X(t)|\mathcal{F}_s] \qquad s < t$$

Furthermore, the following theorem holds

Theorem: The collection $\{X(t) : t \in T\}$ of integrable random variables is a *martingale* iff for all $s, t \in T$ with $s < t$ and all $E \in \mathcal{F}_s$

$$\int_E X(s) dP = \int_E \mathbf{E}[X(t)|\mathcal{F}_s] dP = \int_E X(t) dP$$

and a *semi-martingale* iff for all $s, t \in T$ with $s < t$ and all $E \in \mathcal{F}_s$

$$\int_E X(s) dP \leq \int_E \mathbf{E}[X(t)|\mathcal{F}_s] dP \leq \int_E X(t) dP \qquad \square$$

The relationship between martingales and the Wiener process is given by the following theorem from Doob[38]

Theorem: Let $\{X(t), \mathcal{F}_t, a \leq t \leq b\}$ be a real martingale, and suppose that almost all sample paths of the process are continuous. Suppose that

$$\mathbf{E}[X(t)^2] < \infty \qquad a \leq t \leq b$$

and that for each pair s, t with $s < t$

$$\mathbf{E}[(X(t) - X(s))^2]|\mathcal{F}_s] = t - s$$

with probability 1. Then it follows that the $X(t)$ process has independent increments and is a Wiener process. $\square$

Doob[38] defines the stochastic integral

$$\int_E \Phi(t,\omega)d\beta(t)$$

by assuming that the process $\beta(t)$ is a martingale. An extension of the theory to semimartingales can be found in Protter[81]. The Itô integral follows as a special case from the preceding theorem.

Jazwinski[56] defines the Itô integral as the mean square limit of step function processes in the following manner:

Definition A *step function*, $g(t,\omega)$, is defined as

$$g(t,\omega) = \begin{cases} 0 & t < a_1 \\ g_j(\omega) & a_j \le t < a_{j+1} \quad j \le n-1 \\ 0 & a_n \le t \end{cases}$$

where $a_1 < \cdots < a_n$, and $g_j(\omega)$ is measurable with respect to $\mathcal{F}_{a_j}$ and $E\left[|g_j(\omega)|^2\right] < \infty$ and $g_j(\omega)$ is independent of

$$\{\beta(a_k) - \beta(a_l) : a_j \le a_l \le a_k \le a_n\}$$

This is a condition of *nonanticipativeness.* One way of interpreting this is that the function g_j is independent of the Wiener process in future time t. In other words, the values of g_j are observable only by events prior to a_j.

Let $\{g^n(t,\omega)\}$ be a sequence of step function processes converging to the process $g(t,\omega)$ in the sense that

$$\int_T E\left[|g(t,\omega) - g^n(t,\omega)|^2\right] dt \to 0 \qquad \text{as } n \to \infty$$

then the Itô integral of the process $g(t,\omega)$ with respect to the Wiener process $\beta(t,\omega)$ is defined to be

$$\int_T g(t,\omega)d\beta(t) = (m^2) \lim_{n\to\infty} \int_T g^n(t,\omega)d\beta(t)$$

Stochastic integrals are defined in the sense of mean squared convergence which implies convergence in measure P, because if $\epsilon > 0$ and

$$\Omega_n = \left\{\omega : \left| \int_T g^n(t,\omega)d\beta(t) - \int_T g(t,\omega)d\beta(t) \right| \ge \epsilon \right\}$$

then

$$\int_{\Omega_n} \left| \int_T g^n(t,\omega)d\beta(t) - \int_T g(t,\omega)d\beta(t) \right|^2 dP \ge \int_{\Omega_n} \epsilon^2 dP = \epsilon^2 P(\Omega_n)$$

Hence, from the mean convergence it follows that

$$
\begin{aligned}
P(\Omega_n) &\leq \frac{1}{\epsilon^2}\int_{\Omega_n}\left|\int_T g^n(t,\omega)d\beta(t) - \int_T g(t,\omega)d\beta(t)\right|^2 dP \\
&\leq \frac{1}{\epsilon^2}\int_{\Omega}\left|\int_T g^n(t,\omega)d\beta(t) - \int_T g(t,\omega)d\beta(t)\right|^2 dP \\
&\to 0 \quad \text{as } n \to \infty
\end{aligned}
$$

In order to extend these results to a Hilbert space, H, it is necessary to define a Wiener process in a Hilbert space, Falb[39], Curtain and Falb[26], [27], and Sawaragi, Soeda, Omatu[90]. If $W(t)$ is an H-valued Wiener process, then there are complex random processes $\{\beta_i\}_{i=0}^{\infty}$ such that

$$
W(t) = \sum_{i=0}^{\infty} \beta_i(t)e_i
$$

almost everywhere in (t,ω). Here, $\{e_i\}_{i=0}^{\infty}$ is an orthonormal basis of H. And, $\Re(\beta_i(t))$ and $\Im(\beta_i(t))$ are real Wiener processes.

Itô stochastic integration is extended to the Hilbert space setting as follows: First, in Section 1.3, a complex-valued second order random variable was defined in terms of the modulus function, $|\cdot|$. In the case of a Hilbert space valued random variable, the H-valued random variable, $X(\omega)$, is second order if

$$
\mathbf{E}\left[\|X(\omega)\|_H^2\right] < \infty
$$

where the modulus function is now replaced by the H-norm, $\|\cdot\|_H$. Secondly, the mean squared convergence is done in terms of the $\|\cdot\|_H$ norm instead of the $|\cdot|$ function.

Let H be a Hilbert space and $W(t)$ an H-valued Wiener process. Also, let $g(t,\omega)$ be a step function from T into $\mathcal{L}(H,H)$

$$
g(t,\omega) = \begin{cases} 0 & t < a_1 \\ g_j(\omega) & a_j \leq t < a_{j+1} \quad j \leq n-1 \\ 0 & a_n \leq t \end{cases}
$$

where $a_1 < \cdots < a_n$, and if $g^n(t,\omega)$ is a sequence of step functions converging to $g(t,\omega)$, then

$$
\begin{aligned}
\int_T g(t,\omega)dW(t) &= (m^2)\lim_{n\to\infty}\int_T g^n(t,\omega)dW(t) \\
&= (m^2)\lim_{n\to\infty}\sum_{j=1}^{n} g_j^n(\omega)\left[W(t_j) - W(t_{j-1})\right]
\end{aligned}
$$

Or,

$$
\lim_{n\to\infty}\mathbf{E}\left[\left\|\int_T g^n(t,\omega)dW(t) - \int_T g(t,\omega)dW(t)\right\|_H^2\right] = 0
$$

Because the Itô integral is applicable to a wider class of functions, it is used in this analysis even though new rules of Itô calculus must be devised.

3.5 Itô's Lemma In Hilbert Space

The most important new rule required for the solution of the stochastic evolution equations is Itô's lemma in Hilbert space. It is a kind of change of variable formula. The one-dimensional version of the Itô formula was described in Section 1.1, where the relationship

$$dW(t)^2 = dt$$

was used to develop it. Using the relationship

$$\mathbf{E}\left[d\vec{W}(t)\, d\vec{W}(t)^{\dagger}\right] = Q(t)dt$$

where

$$\vec{W}(t) = \left[W^1(t), \cdots, W^m(t)\right]^{\dagger}$$

is an m-dimensional Wiener process, and the mappings

$$\vec{a} : [t_0, T] \times \Re^d \to \Re^d$$

$$\mathbf{b} : [t_0, T] \times \Re^d \to \Re^{d \times m}$$

the *d-dimensional vector stochastic differential equation* is

$$d\vec{X}(t) = \vec{a}(t, \vec{X}(t)) + \mathbf{b}(t, \vec{X}(t))\, d\vec{W}(t)$$

Then, Jazwinski[56], Kloeden[61], Kloeden, *et al*[62], for a sufficiently smooth function

$$g : [t_0, T] \times \Re^d \to \Re^k$$

of the solution $\vec{X}(t)$, $t_0 \le t \le T$, there is a k-dimensional process

$$\vec{Y}(t) = g(t, \vec{X}(t)) \qquad t_0 \le t \le T$$

such that for the p^{th} component of the vector process $\vec{Y}(t)$,

$$\begin{aligned} dY^p(t) &= \left(\frac{\partial g^p}{\partial t} + \sum_{i=1}^{d} a^i \frac{\partial g^p}{\partial x_i} + \frac{1}{2} \sum_{j,k=1}^{d} \sum_{i,l=1}^{m} b_{ki} Q_{il} b_{jl} \frac{\partial^2 g^p}{\partial x_j\, \partial x_k} \right) dt \\ &+ \sum_{l=1}^{m} \sum_{i=1}^{d} b_{il} \frac{\partial g^p}{\partial x_i}\, dW^l(t) \qquad p = 1, \cdots, k \end{aligned}$$

where all terms are evaluated at the points $(t, \vec{X}(t))$. This is the finite dimensional vector version of Itô's formula.

As for the infinite dimensional version, let

$$\begin{aligned} \mu_1(H, K) &= \{S(t, \omega) : S(t, \omega) \in \mathcal{L}(H, K) \\ &\qquad \textit{and} \int_0^T \mathbf{E}[\|S(t, \omega)\|^2_{\mathcal{L}(H,K)}]dt < \infty\} \end{aligned}$$

Itô's Lemma Let H, K, and G be Hilbert spaces and let $W(t)$ be an H-valued Wiener process. Suppose that $g(t, c)$ is a continuous map of $[0, T] \times K$ into G and that $u(t)$ is a K-valued stochastic process with stochastic differential

$$du(t) = A(t, \omega)dt + C(t, \omega)dW(t)$$

such that

- $g_t(t,c)$ is continuous on $[0,T] \times K$
- $g(t,\cdot)$ is twice continuously differentiable on K for each *fixed* $t \in [0,T]$.
- $g_c(t,c)$ and $g_{cc}(t,c)$ are continuous in (t,c) on $[0,T] \times K$.
- $A(t,\omega)$ is a K-valued stochastic process which is measurable relative to $\mathcal{F}_t$, $t \in [0,T]$, and integrable on $[0,T]$, with probability 1.
- $C(t,\omega) \in \mu_1(H,K)$ and $\int_0^T \mathbf{E}[||C(t,\omega)||^4]dt < \infty$
- $W(t)$ is real, and g_t and g_c denote the partial and Frechet derivatives.

Then

$$z(t) = g(t,u(t))$$

has the G-valued stochastic differential

$$\begin{aligned} dz(t) &= \left\{ g_t(t,u(t)) + g_c(t,u(t))[A(t,\omega)] + \frac{1}{2}\tilde{tr}(g_{cc}(t,u(t))[C(t)\xi_W] \right\} dt \\ &+ g_c(t,u(t))[C(t)]dW(t) \end{aligned}$$

Here $\tilde{tr}$ represents a trace operator which is defined as

$$\tilde{tr}(g_{cc}(t,u(t))[C(t)\xi_W] \equiv \sum_{i=1}^{\infty} g_{cc}(t,u(t))[C(t)\sqrt{\lambda_i}e_i, C(t)\sqrt{\lambda_i}e_i] \tag{14}$$

where $\xi_W = \sum_{i=1}^{\infty} \sqrt{\lambda_i}e_i$ and the $\{e_i\}$ is an orthonormal basis of H of eigenvectors of Q, the covariance operator associated with the Wiener process, $W(t)$, with corresponding eigenvalues $\{\lambda_i\}$. The existence of these eigenvalues and eigenvectors follows from the definition of an H-valued Wiener process, Falb[39], Curtain and Falb[26, 27] and Sawaragi, Soeda and Omatu[90], where the covariance operator, Q, is assumed to be compact.

A Corollary that will be more useful is:

Corollary: Suppose that in addition to the hypothesis of the theorem that we let $G = \Re^1$. Then $dz(t)$ can be written as

$$\begin{aligned} dz(t) &= \{g_t(t,u(t)) + (A(t,\omega), \nabla_c g(t,u(t))) \\ &+ \frac{1}{2}tr(C(t,\omega)Q(t)C^*(t,\omega)\Theta_{cc}g(t,u(t)))\}dt \\ &+ (C^*(t,\omega)\nabla_c g(t,u(t)), dW(t)) \end{aligned}$$

where $\nabla_c g$ and $\Theta_{cc} g$ are the gradient and Hessian of g with respect to c.

Versions of these results on Itô's lemma are found in Curtain and Falb[26], Bensoussan[14] and Sawaragi, Soeda, Omatu[90].

3.6 Small o Notation

Let X be a B-space with dual X', then $< y', x >$ is the duality pairing of y' and x. Let $x_1 \in X$, $y_1' \in X'$ and define the mapping

$$x_1 \circ y_1' : X \to X$$

such that

$$(x_1 \circ y_1')x = x_1 < y_1', x > \qquad \forall x \in X$$

Theorem: Let X be a B-space and let ψ be the mapping of $X \oplus X'$ into $\mathcal{L}(X, X)$ defined by

$$\psi(x_1, y_1') = x_1 \circ y_1'$$

Then ψ has the following properties:

- ψ is continuous
- ψ is linear in both x_1 and y_1'
- $(x_1 \circ y_1')' = y_1' \circ x_1$ if X is reflexive

Note: If $X = \Re^n$, then $\vec{x}_1 \circ \vec{y}_1'$ can be identified with the matrix $\vec{x}_1 \vec{y}_1^{\dagger}$.

The small $\circ$ notation can be used to define the concept of covariance on a Hilbert space H. The inner product $(h, X(\omega))_H$ is a linear random functional on H'. So, if $X(\omega) \in H$, then

$$(\cdot, X(\omega))_H : H' \to \Re^1$$

and $(h, X(\omega))_H$ is a real random variable. Hence, $\mathbf{E}[(h_1, X_1)_H (h_2, X_2)_H]$ represents the covariance of X_1 and X_2. Let $h_1, h_2 \in H'$ and let $X_1, X_2 \in H$, then by identifying $H = H'$ it follows that

$$\begin{aligned} \left(h_1, (X_1 \circ X_2')h_2\right)_H &= (h_1, (X_1 \circ X_2)h_2)_H \\ &= (h_1, X_1(X_2, h_2)_H)_H \\ &= (h_1, X_1)_H \, (h_2, X_2)_H \end{aligned}$$

Since $(X_1 \circ X_2')h_2 \in H$, by taking expectations it follows that

$$\mathbf{E}[(h_1, X_1)_H (h_2, X_2)_H] = \left(h_1, \mathbf{E}[(X_1 \circ X_2')h_2]\right)_H$$

Assuming for the moment that $\mathbf{E}[X_1] = \mathbf{E}[X_2] = 0$ and that the mapping

$$\Xi : H' \times H' \longrightarrow \Re^1 \qquad \ni$$

$$\Xi(h_1, h_2) = \mathbf{E}\left[(h_1, x_1)_H (h_2, x_2)_H\right] = (h_1, \mathrm{Cov}[x_1, x_2]h_2)_H$$

Then, by the Riesz Representation theory, there is a unique Riesz map $\Lambda \in \mathcal{L}(H', H)$ such that

$$\Xi(h_1, h_2) = (h_1, \Lambda h_2)_H$$

where Λ is called the covariance operator, and since Λ is unique, $\Lambda = \mathbf{E}[X_1 \circ X_2']$. In the case that the expected values of X_1 and X_2 are not zero, the covariance operator of X_1 and X_2' is defined as, Falb[39],

$$\mathrm{Cov}[X_1, X_2] = \mathrm{Cov}[X_1, X_2'] = \mathbf{E}[X_1 \circ X_2'] - \mathbf{E}[X_1] \circ \mathbf{E}[X_2']$$

3.7 Hilbert Space Structures

Kadison[57] gives the following definitions for a *Direct Sum Of Hilbert Spaces* and for a *Direct Sum Of Operators*:

Let $\mathcal{H}_1$, $\mathcal{H}_2$, $\cdots$, $\mathcal{H}_n$ be Hilbert spaces and $\mathcal{K}$ be the set of all n-tuples $\{x_1, x_2, \cdots, x_n\}$ with $x_i \in \mathcal{H}_i$. Then there is a Hilbert space structure on $\mathcal{K}$ with the following definitions:

Algebraic Operations:

$$a\{x_1, \cdots, x_n\} + b\{y_1, \cdots, y_n\} = \{ax_1 + by_1 \ \cdots, ay_n + by_n\}$$

Inner Product:

$$< \{x_1, \cdots, x_n\}, \{y_1, \cdots, y_n\} >= (x_1, y_1) + \cdots + (x_n, y_n)$$

Norm:

$$\|\{x_1, \cdots, x_n\}\| = [\|x_1\|^2 + \cdots + \|x_n\|^2]^{\frac{1}{2}}$$

The resulting Hilbert space $\mathcal{K}$ is called a *Hilbert direct sum of* $\mathcal{H}_1, \cdots, \mathcal{H}_n$ and is denoted

$$\mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_n \equiv \sum_{i=1}^{n} \oplus \mathcal{H}_i$$

Let $\mathcal{H}_i$ and $\mathcal{K}_i$ be Hilbert spaces and $T_i \in \mathcal{L}(\mathcal{H}_i, \mathcal{K}_i), i = 1, \cdots, n$, then the equation

$$T\{x_1, \cdots, x_n\} = \{T_1 x_1, \cdots, T_n x_n\} \quad x_1 \in \mathcal{H}_1, \cdots, x_n \in \mathcal{H}_n$$

defines a linear operator T such that

$$T : \sum_{i=1}^{n} \oplus \mathcal{H}_i \rightarrow \sum_{i=1}^{n} \oplus \mathcal{K}_i$$

where

$$T \equiv \sum_{i=1}^{n} \oplus T_i$$

The following notation will be used:

$$\{x_1, \cdots, x_n\} \equiv \sum_{i=1}^{n} \oplus x_i$$

The direct sum of operators has the following properties:

$$\begin{aligned}
\left(\sum_{i=1}^{n} \oplus T_i\right)^* &= \sum_{i=1}^{n} \oplus T_i^* \\
\sum_{i=1}^{n} \oplus (aS_i + bT_i) &= a\left(\sum_{i=1}^{n} \oplus S_i\right) + b\left(\sum_{i=1}^{n} \oplus T_i\right) \\
\left(\sum_{i=1}^{n} \oplus R_i\right)\left(\sum_{i=1}^{n} \oplus S_i\right) &= \sum_{i=1}^{n} \oplus R_i S_i
\end{aligned}$$

Frechet Derivatives

In order to derive the first moment equation, let

$$g(t,\nu) = (h,\nu)_H \qquad h \in H'$$

So that

$$g : [0,T] \times H \to \Re^1$$

And, for a fixed t,

$$g : H \to \Re^1$$

If the Frechet derivative exists, then the Gateaux derivative exists and the two are equal. Denote the Frechet derivative by the symbol

$$\frac{\partial g}{\partial \nu} \in \mathcal{L}(H, \Re^1)$$

By the Riesz Representation theorem, the Frechet derivative can be represented by the inner product on H. So, for a fixed h, the Frechet derivative is defined as

$$\frac{\partial g}{\partial \nu}\eta = \left(\frac{\partial g}{\partial \nu}, \eta\right)_H = \lim_{\epsilon \to 0} \frac{(h, \nu + \alpha\eta)_H - (h,\nu)_H}{\alpha}$$

From this definition it follows that

$$\left(\frac{\partial g}{\partial \nu}, \eta\right)_H = (h,\eta)_H \qquad \Rightarrow \qquad \frac{\partial g}{\partial \nu} = h \in \mathcal{L}(H, \Re^1)$$

Since h and η are fixed, $(h,\eta)_H$ is a constant. So, the second Frechet derivative of g is zero.

To derive the second moment equation, let

$$g(t,\nu) = (h_1,\nu)_H (h_2,\nu)_H$$

Then,

$$\begin{aligned} \left(\frac{\partial g}{\partial \nu}, \eta\right)_H &= \lim_{\epsilon \to 0} \frac{(h_1, \nu + \epsilon\eta)(h_2, \nu + \epsilon\eta) - (h_1,\nu)(h_2,\nu)}{\epsilon} \\ &= \lim_{\epsilon \to 0} \frac{(h_1, \epsilon\eta)(h_2,\nu) + (h_1,\nu)(h_2,\epsilon\eta) + (h_1,\epsilon\eta)(h_2,\epsilon\eta)}{\epsilon} \\ &= (h_1,\eta)(h_2,\nu) + (h_1,\nu)(h_2,\eta) \end{aligned}$$

Or, in operator notation if we let

$$T_1 = (h_1, \cdot)h_2 \qquad \text{and} \qquad T_2 = (h_2, \cdot)h_1$$

Then,

$$T = T_1 \oplus T_2 : H \oplus H \to H \oplus H$$

and, using the definitions for the inner products we have,

$$< (h_1,\nu)h_2 \oplus (h_2,\nu)h_1, \eta \oplus \eta >= (h_1,\eta)(h_2,\nu) + (h_1,\nu)(h_2,\eta) = \left(\frac{\partial g}{\partial \nu}, \eta\right)_H$$

So, we can make the identification

$$\frac{\partial g}{\partial \nu} = (h_1,\nu)h_2 \oplus (h_2,\nu)h_1$$

For the second derivative, we can write

$$\frac{\partial^2 g}{\partial \nu^2} \in \mathcal{L}(H, \mathcal{L}(H, \Re^1)) \cong \mathcal{L}(H \oplus H, \Re^1)$$

where $\cong$ represents an isometry. Again, by the Riesz Representation theorem, the second derivative is given by

$$\begin{aligned}
\frac{\partial^2 g}{\partial \nu^2}(\zeta, \eta) &= \left(\frac{\partial^2 g}{\partial \nu^2} \zeta \oplus \zeta, \eta \oplus \eta \right)_{H \oplus H} \\
&= \lim_{\epsilon \to 0} \frac{[(h_1, \nu + \epsilon\zeta)(h_2, \eta) + (h_2, \nu + \epsilon\zeta)(h_1, \eta)] - [(h_1, \nu)(h_2, \eta) + (h_2, \nu)(h_1, \eta)]}{\epsilon} \\
&= \lim_{\epsilon \to 0} \frac{[(h_1, \nu + \epsilon\zeta)(h_2, \eta) - (h_1, \nu)(h_2, \eta)] + [(h_2, \nu + \epsilon\zeta)(h_1, \eta) - (h_2, \nu)(h_1, \eta)]}{\epsilon} \\
&= (h_1, \zeta)(h_2, \eta) + (h_2, \zeta)(h_1, \eta) \qquad \zeta, \quad \eta \in H
\end{aligned}$$

And, if we identify H with its dual H' we can write this operator in terms of the small o notation, so that

$$(h_1, \zeta)h_2 = (h_2 \circ h_1)\zeta$$

With this notation we can write

$$\begin{aligned}
\frac{\partial^2 g}{\partial \nu^2}(\zeta, \eta) &= (h_1, \zeta)(h_2, \eta) + (h_2, \zeta)(h_1, \eta) \\
&= < (h_2 \circ h_1) \oplus (h_1 \circ h_2)\zeta \oplus \zeta, \eta \oplus \eta >
\end{aligned}$$

Hence,

$$\frac{\partial^2 g}{\partial \nu^2} = h_1 \circ h_2 \oplus h_2 \circ h_1$$

3.8 Moment Equation Derivation

In this section, equations for which the forcing term has a Gaussian white noise component are discussed, References for this section are Bensoussan[14], Chow[22], Kloeden[61] and Serrano, Unny, Lennox[95].

In the finite dimensional case, the general form of a d-dimensional *linear stochastic differential equation* is

$$d\vec{X}_t = \left(\mathbf{A}(t)\vec{X}_t + \vec{a}(t) \right) dt + \sum_{l=1}^{m} \left(\mathbf{B}^l(t)\vec{X}_t + \vec{b}^l(t) \right) dW_t^l$$

where $t \in [0, T]$, $\mathbf{A}(t), \mathbf{B}^1(t), \cdots, \mathbf{B}^m(t)$ are $d \times d$-matrix functions and $\vec{a}(t), \vec{b}^1(t), \cdots, \vec{b}^m(t)$ are d-dimensional vector functions, Kloeden[61].

This equation is to be interpreted in its integral form as

$$\vec{X}_t = \vec{X}_0 + \int_0^t \left(\mathbf{A}(s)\vec{X}_s + \vec{a}(s) \right) ds + \sum_{l=1}^{m} \int_0^t \left(\mathbf{B}^l(s)\vec{X}_s + \vec{b}^l(s) \right) dW_s^l$$

Taking expectations and using the zero expected value property of the Itô's integral, it follows that

$$\mathbf{E}[\vec{X}_t] = \mathbf{E}[\vec{x}_0] + \int_0^t \left(\mathbf{A}(s)\mathbf{E}[\vec{X}_s] + \vec{a}(s)\right) ds$$

which in differential form is

$$\boxed{\frac{d\mathbf{E}[\vec{X}_t]}{dt} = \mathbf{A}(t)\mathbf{E}[\vec{X}_t] + \vec{a}(t)}$$

In order to establish a differential equation for the $\mathbf{E}[\vec{X}_t \vec{X}_t^T]$, Itô's formula is used, which states that for a sufficiently smooth mapping

$$U : [0, T] \times \Re^d \to \Re^k$$

of the solution process $\vec{X}_t$, we obtain a k-dimensional process

$$\vec{Y}_t = U(t, \vec{X}_t)$$

then

$$\begin{aligned} dY_t^p &= \left(\frac{\partial U^p}{\partial t} + \sum_{i=1}^{d} e_t^i \frac{\partial U^p}{\partial x_i} + \frac{1}{2} \sum_{i,j=1}^{d} \sum_{l=1}^{m} f_t^{i,l} f_t^{j,l} \frac{\partial^2 U^p}{\partial x_i \partial x_j} \right) dt \\ &+ \sum_{l=1}^{m} \sum_{i=1}^{d} f_t^{i,l} \frac{\partial U^p}{\partial x_i} dW_t^l \end{aligned}$$

for $p = 1, 2, \cdots, k$ and all terms are evaluated at $(t, \vec{X}_t)$.

The linear stochastic differential equation

$$d\vec{X}_t = \left(\mathbf{A}(t)\vec{X}_t + \vec{a}(t)\right) dt + \sum_{l=1}^{m} \left(\mathbf{B}^l(t)\vec{X}_t + \vec{b}^l(t)\right) dW_t^l$$

can be rewritten by letting

$$e_t^i = \left(\mathbf{A}(t)\vec{X}_t + \vec{a}(t)\right)^i$$

and expanding the term

$$\sum_{l=1}^{m} \left(\mathbf{B}^l(t)\vec{X}_t + \vec{b}^l(t)\right) dW_t^l$$

where $\mathbf{B}^l(t)$ is $d \times d$, $\vec{X}_t$ and $\vec{b}^l(t)$ are d-dimensional and W_t^l is a scalar Wiener process for $l = 1, \cdots, m$.

Hence, $\forall\, l,\ l = 1, \cdots, m$

$$\begin{aligned} \left(\mathbf{B}^l(t)\vec{X}_t\right)_j &= \sum_{i=1}^{d} B_j^{i,l}(t) X_t^i \qquad j = 1, \cdots, d \\ &\equiv c_j^l(t) \end{aligned}$$

so that

$$\sum_{l=1}^{m}\left(\left(\mathbf{B}^l(t)\vec{X}_t\right)_j + b_j^l(t)\right) dW_t^l = \sum_{l=1}^{m}\left(c_j^l(t) + b_j^l(t)\right) dW_t^l$$
$$\equiv \sum_{l=1}^{m} f_t^{j,l} dW_t^l$$

where

$$f_t^{j,l} = \sum_{i=1}^{d} B_j^{i,l} X^i + b_j^l$$

So, the original SDE can be written in component form as

$$dX_t^j = e_t^j\, dt + \sum_{l=1}^{m} f_t^{j,l}\, dW_t^l \qquad j = 1, \cdots, d$$

Letting $m = 1$ and applying Itô's formula with $U(t,\vec{x}) = \vec{x}\vec{x}^T$ yields the following differential equation for the second moment $\mathbf{E}[\vec{X}\vec{X}^T]$

$$\boxed{\begin{aligned} \frac{d\mathbf{E}[\vec{X}\vec{X}^T]}{dt} &= \mathbf{A}(t)\mathbf{E}[\vec{X}\vec{X}^T] + \mathbf{E}[\vec{X}\vec{X}^T]\mathbf{A}^T(t) \\ &+ \vec{a}(t)\mathbf{E}[\vec{X}]^T + \mathbf{E}[\vec{X}]\vec{a}(t)^T \\ &+ \mathbf{B}\mathbf{E}[\vec{X}\vec{X}^T]\mathbf{B}^T + \vec{b}\mathbf{E}[\vec{X}]^T\mathbf{B} + \mathbf{B}\mathbf{E}[\vec{X}]\vec{b}^T + \vec{b}\vec{b}^T \end{aligned}} \tag{15}$$

A result similar to this will now be derived for the infinite dimensional case. Consider the equation

$$\frac{du}{dt} = -Au + f + \zeta$$

where u is a function of (t, x, ω) and belongs to a Hilbert space H; A is a spatially elliptic operator; f is deterministic; and ζ is a Gaussian white noise process.

In integral form, this equation is

$$u(t) = u(0) + \int_0^t (-Au + f)ds + \int_0^t \zeta(s)ds$$

Then, $W(t) = \int_0^t \zeta(s)ds$ is an H-valued Wiener process and the original equation can be written as

$$du(t) = (-Au + f)dt + dW(t)$$

For more generality, introduce the stochastic operator $\Gamma(t)$ such that $\Gamma(t) \in \mathcal{L}(H, H)$ and

$$\int_0^t \|\Gamma(s)\|^2_{\mathcal{L}(H,H)} ds < \infty$$

So that we have

$$du(t) = (-Au + f)dt + \Gamma(t)dW(t)$$

Using Itô's lemma,

$$\begin{aligned} dg(t,u(t)) &= \left\{ \frac{\partial g}{\partial t}(t,u(t)) + \left(-Au + f, \frac{\partial g}{\partial u}(t,u(t)) \right) \right. \\ &+ \left. \frac{1}{2} tr \Gamma Q(t) \Gamma^* \frac{\partial^2 g}{\partial u^2} \right\} dt + \left(\frac{\partial g}{\partial u}, \Gamma dW \right) \end{aligned} \tag{16}$$

And, $Q(t) \in \mathcal{L}^\infty(0,T;\mathcal{L}(H,H))$ and is called the *covariance operator*.

Allowing $g(0,u(0)) = 0$, Equation[16] can be interpreted in the stochastic differential equation sense as

$$\begin{aligned} g(t,u(t)) &= \int_0^t \left\{ \frac{\partial g}{\partial s}(s,u(s)) + \left(-Au + f, \frac{\partial g}{\partial u}(s,u(s)) \right) \right. \\ &+ \left. \frac{1}{2} tr \Gamma Q(s) \Gamma^* \frac{\partial^2 g}{\partial u^2} \right\} ds + \int_0^t \left(\frac{\partial g}{\partial u}(s,u(s)), \Gamma dW(s) \right) \end{aligned}$$

where $dW(s)$ is to be interpreted as a Gaussian white noise.

Now, if $g = (h,u(t))_H$, $h \in H'$, we have from the Frechet derivative

$$\frac{\partial g}{\partial u} = h \qquad \frac{\partial^2 g}{\partial u^2} = 0$$

Furthermore, since g depends on t only through u,

$$\frac{\partial g}{\partial t} = 0$$

Taking expectations and using the result that $\mathbf{E}[(h,u)_H] = (h,\mathbf{E}[u])_H$, it follows that

$$(h,\mathbf{E}[u])_H = \int_0^t \mathbf{E}\left[(-Au+f,h)_H\right] ds + \int_0^t \mathbf{E}\left[(h,\Gamma dW(s))_H\right]$$

To evaluate the last integral,

$$\begin{aligned} \int_0^t \mathbf{E}[(h,\Gamma dW(s))_H] &= (m^2) \lim_{n\to\infty} \sum_{j=1}^n \mathbf{E}\left[\left(h, g_j^n(\omega)[W(t_{j+1}) - W(t_j)\right)_H \right] \\ &= 0 \end{aligned}$$

since $g_j^n(\omega)$ and $W(t_{j+1}) - W(t_j)$ are independent which follows from the nonanticipativeness of the operator $g_j^n(\omega)$ with respect to $W(t_{j+1}) - W(t_j)$. So, if $M_1 = \mathbf{E}[u]$, then assuming that A is deterministic

$$\left(h, \frac{dM_1}{dt} \right) = -(h, AM_1) + (h,f) \tag{17}$$

Or, in this weak sense, the *first moment equation* is

$$\frac{dM_1}{dt} = -AM_1 + f$$

To obtain the moment equation for the second moment, let

$$g = (h_1,u)_H (h_2,u)_H$$

From the Frechet derivatives we have

$$\frac{\partial g}{\partial u} = (h_1, u)h_2 \oplus (h_2, u)h_1$$

And,

$$\frac{\partial^2 g}{\partial u^2} = h_2 \circ h_1 \oplus h_1 \circ h_2$$

Hence, it follows from Itô's lemma

$$\begin{aligned} \frac{d}{dt}(h_1, u)(h_2, u) &= -< (h_1, u)h_2 \oplus (h_2, u)h_1, Au \oplus Au > \\ &+ < (h_1, u)h_2 \oplus (h_2, u)h_1, f \oplus f > \\ &+ \frac{1}{2} tr[\Gamma^*(h_2 \circ h_1) \oplus (h_1 \circ h_2)\Gamma Q(t)] \\ &+ < (h_1, u)h_2 \oplus (h_2, u)h_1, \Gamma dW \oplus \Gamma dW > \end{aligned}$$

Expanding this equation we get

$$\begin{aligned} \frac{d}{dt}(h_1, u)(h_2, u) &= -[(h_1, u)(h_2, Au) + (h_2, u)(h_1, Au)] \\ &+ (h_1, u)(h_2, f) + (h_2, u)(h_1, f) \\ &+ \frac{1}{2} tr[\Gamma^*(h_2 \circ h_1) \oplus (h_1 \circ h_2)\Gamma Q(t)] \\ &+ (h_1, u)(h_2, \Gamma dW) + (h_2, u)(h_1, \Gamma dW) \end{aligned} \tag{18}$$

Taking expectations and using the following definition of the correlation operator,

$$\mathbf{E}[(h_1, X(\omega))(h_2, Y(\omega))] = (h_1, R_{XY} h_2)$$

where $R_{XY} = M_2$, if $X = Y$, it follows that for $M_2 = M_2^*$ and A deterministic,

$$\begin{aligned} \mathbf{E}[(h_1, u)(h_2, Au)] &= \mathbf{E}[(h_1, u)(A^* h_2, u)] = (h_1, M_2 A^* h_2) \\ \mathbf{E}[(h_2, u)(h_1, Au)] &= \mathbf{E}[(h_2, u)(A^* h_1, u)] = (h_2, M_2 A^* h_1) = (h_1, A M_2 h_2) \\ \mathbf{E}[(h_1, u)(h_2, f)] &= (h_1, R_{uf} h_2) = (h_1, M_1 f h_2) \end{aligned}$$

And,

$$\begin{aligned} \frac{d}{dt}(h_1, M_2 h_2) &= -[(h_1, M_2 A^* h_2) + (h_1, A M_2 h_2)] \\ &+ (h_1, M_1 f h_2) + (h_1, M_1 f h_2) \\ &+ \frac{1}{2}\mathbf{E}\left[tr \Gamma^*(h_2 \circ h_1) \oplus (h_1 \circ h_2)\Gamma Q(t)\right] \end{aligned} \tag{19}$$

Interchanging the roles of h_1 and h_2, we get

$$\begin{aligned} \frac{d}{dt}(h_2, M_2 h_1) &= -[(h_2, M_2 A^* h_1) + (h_2, A M_2 h_1)] \\ &+ (h_2, M_1 f h_1) + (h_2, M_1 f h_1) \\ &+ \frac{1}{2}\mathbf{E}\left[tr \Gamma^*(h_1 \circ h_2) \oplus (h_2 \circ h_1)\Gamma Q(t)\right] \end{aligned} \tag{20}$$

Adding these Equations [19] and [20] together and using the definition of the inner product on a direct sum of Hilbert spaces,

$$
\begin{aligned}
\left\langle h_1 \oplus h_2, \frac{dM_2}{dt} \oplus \frac{dM_2}{dt} h_2 \oplus h_1 \right\rangle &= \langle h_1 \oplus h_2, -(AM_2 \oplus M_2 A^*) h_2 \oplus h_1 \rangle \\
&+ \langle h_1 \oplus h_2, (M_1 f \oplus (M_1 f)^*) h_2 \oplus h_1 \rangle \\
&+ \frac{1}{2} \mathbf{E} \left[tr \Gamma^* (h_2 \circ h_1) \oplus (h_1 \circ h_2) \Gamma Q(t) \right] \\
&+ \frac{1}{2} \mathbf{E} \left[tr \Gamma^* (h_1 \circ h_2) \oplus (h_2 \circ h_1) \Gamma Q(t) \right]
\end{aligned}
$$

where, as before, the last term of Equation[18] vanishes on taking expectations.

Even though this equation has a weak sense formulation, it has a form similar to the simpler case Equation[15], page 20, above. Using Equation[14], page 14, and the fact that $Qe_i = \lambda_i e_i$, the trace term can be put into a more usable form by expanding and using Parseval's relation and the definition of the small o notation

$$
\begin{aligned}
&\frac{1}{2} \tilde{tr} \left(\frac{\partial^2 g}{\partial u^2} \right) [\Gamma \xi_W] = \frac{1}{2} \sum_{i=1}^{\infty} \frac{\partial^2 g}{\partial u^2} \left[\Gamma \sqrt{\lambda_i} e_i, \Gamma \sqrt{\lambda_i} e_i \right] \\
&= \frac{1}{2} \sum_{i=1}^{\infty} (h_1 \circ h_2) \oplus (h_2 \circ h_1) \left[\Gamma \sqrt{\lambda_i} e_i, \Gamma \sqrt{\lambda_i} e_i \right] \\
&= \frac{1}{2} \sum_{i=1}^{\infty} \left[(h_1, \Gamma \sqrt{\lambda_i} e_i) + (h_2, \Gamma \sqrt{\lambda_i} e_i)(h_2, \Gamma \sqrt{\lambda_i} e_i)(h_1, \Gamma \sqrt{\lambda_i} e_i) \right] \\
&= \frac{1}{2} \sum_{i=1}^{\infty} \left[(\Gamma^* h_1, \lambda_i e_i)(\Gamma^* h_2, e_i) + (\Gamma^* h_2, \lambda_i e_i)(\Gamma^* h_1, e_i) \right] \\
&\overset{\text{Parseval}}{=} \frac{1}{2} \left[(Q \Gamma^* h_1, \Gamma^* h_2) + (Q \Gamma^* h_2, \Gamma^* h_1) \right] \\
&= (h_1, \Gamma Q \Gamma^* h_2) \qquad (21)
\end{aligned}
$$

This theory will be demonstrated in the next two examples. The first example will use the theory to derive the mean concentration equation, Equation[4], page 2, the velocity-concentration equation, Equation[7], page 3, and the concentration-covariance equation, Equation[10], page 4. Consider the transport equation

$$
\frac{\partial c}{\partial t} + \nabla \cdot (c \vec{V}) - \nabla \cdot (\mathbf{D} \nabla c) = 0
$$

Suppose that the tensor $\mathbf{D}$ has been specified in a deterministic manner, and the velocity and concentration are expressed as

$$
\vec{V}(\vec{x}, \omega) = \mathbf{E}[\vec{V}(\vec{x})] + \vec{V}'(\vec{x}) \quad ; \quad \mathbf{E}[\vec{V}'(\vec{x})] = 0
$$

$$
c(\vec{x}, t) = \mathbf{E}[c(\vec{x}, t)] + c'(\vec{x}, t) \quad ; \quad \mathbf{E}[c'(\vec{x}, t)] = 0
$$

In terms of Equation[12], page 6,

$$
\begin{aligned}
A(\vec{x}, t, \omega) &= \nabla \cdot ((\cdot)(\mathbf{E}[\vec{V}(\vec{x}, \omega)] + \vec{V}'(\vec{x}, \omega))) - \nabla \cdot (\mathbf{D} \nabla (\cdot)) \\
g(\vec{x}, t, \omega) &= 0
\end{aligned}
$$

From now on, ω will not be specifically stated. Then, from Equation[17] page 21,

$$
\begin{aligned}
\left(h, \frac{\partial c}{\partial t}\right) &= -(h, Ac) \\
&= -\left(h, \nabla \cdot \left[(\mathbf{E}[c] + c')(\mathbf{E}[\vec{V}] + \vec{V'})\right] - \nabla \cdot (\mathbf{D}\nabla(\mathbf{E}[c] + c'))\right) \\
&= -\left(h, \nabla \cdot \left[(\mathbf{E}[c]\mathbf{E}[\vec{V}] + \mathbf{E}[c]\vec{V'} + c'\mathbf{E}[\vec{V}] + c'\vec{V'}\right] - \nabla \cdot (\mathbf{D}\nabla(\mathbf{E}[c] + c'))\right)
\end{aligned}
$$

Taking expectations, and using $\mathbf{E}[c'] = \mathbf{E}[\vec{V'}] = 0$,

$$
\left(h, \frac{\partial \mathbf{E}[c]}{\partial t}\right) = -\left(h, \nabla \cdot \left[(\mathbf{E}[c]\mathbf{E}[\vec{V}] + \mathbf{E}[c'\vec{V'}]\right] - \nabla \cdot (\mathbf{D}\nabla(\mathbf{E}[c]))\right)
$$

So that in the weak sense,

$$
\frac{\partial \mathbf{E}[c]}{\partial t} + \nabla \cdot (\mathbf{E}[c]\mathbf{E}[\vec{V}]) - \nabla \cdot (\mathbf{D}\nabla\mathbf{E}[c]) + \nabla \cdot \mathbf{E}[c'\vec{V'}] = 0
$$

which agrees with Equation[4], page 2. For the second moment equations, let $\vec{x}$ and $\vec{x'}$ be two different coordinate systems, then from Equation[18], page 22, with $h_1,\, h_2 \in H'$,

$$
\begin{aligned}
\frac{\partial}{\partial t}(h_1, c(\vec{x}, t))(h_2, c(\vec{x'}, t)) = -\Big[&(h_1, c(\vec{x}, t))(h_2, A_{\vec{x'}} c(\vec{x'}, t)) \\
&+(h_2, c(\vec{x'}, t))(h_1, A_{\vec{x}} c(\vec{x}, t)\Big] \\
= (h_1, c(\vec{x}, t)) \left(h_2, \frac{\partial c(\vec{x'}, t)}{\partial t}\right) &+ (h_2, c(\vec{x'}, t)) \left(h_1, \frac{\partial c(\vec{x}, t)}{\partial t}\right)
\end{aligned} \tag{22}
$$

as would be expected since the Wiener process is excluded from playing a role in this example. Expanding the left hand side of Equation[22], taking expectations, using $\mathbf{E}[c'(\vec{x}, t)] = \mathbf{E}[c'(\vec{x'}, t)] = 0$ and letting $C_{cc}(\vec{x}, \vec{x'}, t) = \mathbf{E}[c'(\vec{x}, t)c'(\vec{x'}, t)]$

$$
\begin{aligned}
\mathbf{E}\left[\frac{\partial}{\partial t}(h_1, c(\vec{x}, t))(h_2, c(\vec{x'}, t))\right] &= \mathbf{E}\Big[\frac{\partial}{\partial t}(h_1, \mathbf{E}[c(\vec{x}, t)] + c'(\vec{x}, t)]) \\
&\qquad \times (h_2, \mathbf{E}[c(\vec{x'}, t)] + c'(\vec{x'}, t))\Big] \\
&= \frac{\partial}{\partial t}\left[\mathbf{E}(h_1, \mathbf{E}[c(\vec{x}, t)])(h_2, \mathbf{E}[c(\vec{x'}, t)]) + (h_1, C_{cc}(\vec{x}, \vec{x'}, t)h_2)\right] \\
&= \frac{\partial}{\partial t}\left[(h_1, \mathbf{E}[c(\vec{x}, t)]\mathbf{E}[c(\vec{x'}, t)]h_2) + (h_1, C_{cc}(\vec{x}, \vec{x'}, t)h_2)\right] \\
&= \left(h_1, \frac{\partial \mathbf{E}[c(\vec{x}, t)]}{\partial t}\mathbf{E}[c(\vec{x'}, t)]h_2\right) + \left(h_1, \frac{\partial \mathbf{E}[c(\vec{x'}, t)]}{\partial t}\mathbf{E}[c(\vec{x}, t)]h_2\right) \\
&\qquad + \frac{\partial}{\partial t}(h_1, C_{cc}(\vec{x}, \vec{x'}, t)h_2)
\end{aligned}
$$

Setting this equal to the expected value of the right hand side of Equation[22]

$$
\begin{aligned}
&\frac{\partial}{\partial t}\left(h_1, C_{cc}(\vec{x}, \vec{x'}, t)h_2\right) + \left(h_1, \mathbf{E}\left[\frac{\partial \mathbf{E}[c(\vec{x}, t)]}{\partial t}c(\vec{x'}, t) + \frac{\partial \mathbf{E}[c(\vec{x'}, t)]}{\partial t}c(\vec{x}, t)\right] h_2\right) \\
&\quad = \left(h_1, \mathbf{E}\left[\frac{\partial c(\vec{x'}, t)}{\partial t}c(\vec{x}, t)\right] h_2\right) + \left(h_1, \mathbf{E}\left[\frac{\partial c(\vec{x}, t)}{\partial t}c(\vec{x'}, t)\right] h_2\right)
\end{aligned}
$$

so that on rearranging terms,

$$\begin{aligned}\frac{\partial}{\partial t}(h_1, C_{cc}(\vec{x},\vec{x'},t)h_2) &= -\left(h_1, \mathbf{E}\left[c(\vec{x'},t)A_{\vec{x}}c(\vec{x},t) + \frac{\partial \mathbf{E}[c(\vec{x},t)]}{\partial t}c(\vec{x'},t)\right] h_2\right) \\ &- \left(h_1, \mathbf{E}\left[c(\vec{x},t)A_{\vec{x'}}c(\vec{x'},t) + \frac{\partial \mathbf{E}[c(\vec{x'},t)]}{\partial t}c(\vec{x},t)\right] h_2\right)\end{aligned} \tag{23}$$

From the first moment equation,

$$\frac{\partial \mathbf{E}[c(\vec{x},t)]}{\partial t} = -\nabla_{\vec{x}}\cdot(\mathbf{E}[c(\vec{x},t)]\mathbf{E}[\vec{V}(\vec{x})]) + \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}\mathbf{E}[c(\vec{x},t)]) - \nabla_{\vec{x}}\cdot\mathbf{E}[c'(\vec{x},t)\vec{V'}(\vec{x})]$$

and,

$$\begin{aligned}\frac{\partial \mathbf{E}[c(\vec{x'},t)]}{\partial t} = -\nabla_{\vec{x'}}\cdot(\mathbf{E}[c(\vec{x'},t)]\mathbf{E}[\vec{V}(\vec{x'})]) &+ \nabla_{\vec{x'}}\cdot(\mathbf{D}\nabla_{\vec{x'}}\mathbf{E}[c(\vec{x'},t)]) \\ &- \nabla_{\vec{x'}}\cdot\mathbf{E}[c'(\vec{x'},t)\vec{V'}(\vec{x'})]\end{aligned}$$

Since

$$A_{\vec{x}}(\cdot) = \nabla_{\vec{x}}\cdot((\cdot)(\mathbf{E}[\vec{V}(\vec{x})] + \vec{V'}(\vec{x})) - \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}(\cdot))$$

it follows from the first term on the right hand side of Equation[23] and by letting $c(\vec{x},t) = \mathbf{E}[c(\vec{x},t)] + c'(\vec{x},t)$ that

$$\begin{aligned}&- \left(h_1, \mathbf{E}\left[c(\vec{x'},t)A_{\vec{x}}c(\vec{x},t) + \frac{\partial \mathbf{E}[c(\vec{x},t)]}{\partial t}c(\vec{x'},t)\right] h_2\right) \\ &= -\Big(h_1, \mathbf{E}\Big[c(\vec{x'},t)\Big[\nabla_{\vec{x}}\cdot(\mathbf{E}[c(\vec{x},t)]\vec{V'}(\vec{x}) + c'(\vec{x},t)\mathbf{E}[\vec{V}(\vec{x})] \\ &+ c'(\vec{x},t)\vec{V'}(\vec{x})) - \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}c'(\vec{x},t)) - \nabla_{\vec{x}}\cdot\mathbf{E}[c'(\vec{x},t)\vec{V'}(\vec{x})]\Big]\Big] h_2\Big)\end{aligned}$$

letting $c(\vec{x'},t) = \mathbf{E}[c(\vec{x'},t)] + c'(\vec{x'},t)$ and expanding the previous result,

$$\begin{aligned}&= -\Big(h_1, \mathbf{E}\Big[\nabla_{\vec{x}}\cdot\Big(\mathbf{E}[c(\vec{x'},t)]\mathbf{E}[c(\vec{x},t)]\vec{V'}(\vec{x}) + c'(\vec{x'},t)\mathbf{E}[c(\vec{x},t)]V'(\vec{x}) \\ &+ \mathbf{E}[c(\vec{x'},t)]c'(\vec{x},t)\mathbf{E}[\vec{V}(\vec{x})] + c'(\vec{x'},t)c'(\vec{x},t)\mathbf{E}[\vec{V}(\vec{x})] \\ &+ \mathbf{E}[c(\vec{x'},t)]c'(\vec{x},t)\vec{V'}(\vec{x}) + c'(\vec{x'},t)c'(\vec{x},t)\vec{V'}(\vec{x})) \\ &- \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}c'(\vec{x},t)\mathbf{E}[c(\vec{x'},t)]) - \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}c'(\vec{x},t)c'(\vec{x'},t))\Big) \\ &- \nabla_{\vec{x}}\cdot\mathbf{E}[c'(\vec{x},t)\vec{V'}(\vec{x})]\mathbf{E}[c(\vec{x'},t)] - \nabla_{\vec{x}}\cdot\mathbf{E}[c'(\vec{x},t)\vec{V'}(\vec{x})]c'(\vec{x'},t)\Big] h_2\Big)\end{aligned}$$

taking expectations, cancelling terms and using $\mathbf{E}[c'] = \mathbf{E}[\vec{V'}] = 0$

$$\begin{aligned}&= -\Big(h_1, \Big[\nabla_{\vec{x}}\cdot\mathbf{E}[c(\vec{x},t)]C_{c\vec{V}}(\vec{x},\vec{x'},t) + \nabla_{\vec{x}}\cdot\mathbf{E}[\vec{V}(\vec{x})]C_{cc}(\vec{x},\vec{x'},t) \\ &+ \nabla_{\vec{x}}\cdot\mathbf{E}[c'(\vec{x'},t)c'(\vec{x},t)\vec{V'}(\vec{x})] - \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}C_{cc}(\vec{x},\vec{x'},t))\Big] h_2\Big)\end{aligned} \tag{24}$$

Also, from the second term on the right hand side of Equation[23] an equation exactly like this one can be derived in the same way only with the vectors $\vec{x}$ and $\vec{x'}$ interchanged.

$$
\begin{aligned}
- & \left(h_1, \left[\nabla_{\vec{x'}} \cdot \mathbf{E}[c(\vec{x'},t)]C_{c\vec{V}}(\vec{x'},\vec{x},t) + \nabla_{\vec{x'}} \cdot \mathbf{E}[\vec{V}(\vec{x'})]C_{cc}(\vec{x'},\vec{x},t)\right.\right. \\
+ & \left.\left. \nabla_{\vec{x'}} \cdot \mathbf{E}[c'(\vec{x},t)c'(\vec{x'},t)\vec{V}'(\vec{x'})] - \nabla_{\vec{x'}} \cdot (\mathbf{D}\nabla_{\vec{x'}} C_{cc}(\vec{x'},\vec{x},t))\right] h_2\right)
\end{aligned} \tag{25}
$$

Equations[23], [24] and [25] give the result for the concentration covariance equation as

$$
\begin{aligned}
\frac{\partial}{\partial t}(h_1, C_{cc}(\vec{x},\vec{x'},t)h_2) = & - \left(h_1, \left[\nabla_{\vec{x}} \cdot \mathbf{E}[c(\vec{x},t)]C_{c\vec{V}}(\vec{x},\vec{x'},t) + \nabla_{\vec{x}} \cdot \mathbf{E}[\vec{V}(\vec{x})]C_{cc}(\vec{x},\vec{x'},t)\right.\right. \\
& \left.\left. + \nabla_{\vec{x}} \cdot \mathbf{E}[c'(\vec{x'},t)c'(\vec{x},t)\vec{V}'(\vec{x})] - \nabla_{\vec{x}} \cdot (\mathbf{D}\nabla_{\vec{x}} C_{cc}(\vec{x},\vec{x'},t))\right] h_2\right) \\
& - \left(h_1, \left[\nabla_{\vec{x'}} \cdot \mathbf{E}[c(\vec{x'},t)]C_{c\vec{V}}(\vec{x'},\vec{x},t) + \nabla_{\vec{x'}} \cdot \mathbf{E}[\vec{V}(\vec{x'})]C_{cc}(\vec{x'},\vec{x},t)\right.\right. \\
& \left.\left. + \left[\nabla_{\vec{x'}} \cdot \mathbf{E}[c'(\vec{x},t)c'(\vec{x'},t)\vec{V}'(\vec{x'})] - \nabla_{\vec{x'}} \cdot (\mathbf{D}\nabla_{\vec{x'}} C_{cc}(\vec{x'},\vec{x},t))\right] h_2\right)
\end{aligned}
$$

Comparing this with Equation[10], page 4, it is seen that this equation is the vector form of Equation[10].

Finally, returning to Equation[17], page 21, and multiplying both sides by $(h, \vec{V}_i(\vec{x'})$, where $\vec{V}_i(\vec{x'})$ is the i^{th} compoment of the vector $\vec{V}(\vec{x'})$, we have

$$
\frac{\partial}{\partial t}(h_1, c(\vec{x},t))(h_2, \vec{V}_i(\vec{x'})) = - \left[(h_1, A_{\vec{x}} c(\vec{x},t))(h_2, \vec{V}_i(\vec{x'}))\right]
$$

Next, write

$$
\begin{aligned}
\frac{\partial}{\partial t}(h_1, c'(\vec{x},t))(h_2, \vec{V'}_i(\vec{x'}) = & \frac{\partial}{\partial t}(h_1, c(\vec{x},t) - \mathbf{E}[c(\vec{x},t)])(h_2, \vec{V}_i(\vec{x'}) - \mathbf{E}[\vec{V}_i(\vec{x'})]) \\
= & \frac{\partial}{\partial t}\left[(h_1, c(\vec{x},t))(h_2, \vec{V}_i(\vec{x'})) - (h_1, c(\vec{x},t))(h_2, \mathbf{E}[\vec{V}_i(\vec{x'})])\right. \\
& \left. - (h_1, \mathbf{E}[c(\vec{x},t)])(h_2, \vec{V}_i(\vec{x'})) + (h_1, \mathbf{E}[c(\vec{x},t)])(h_2, \mathbf{E}[\vec{V}_i(\vec{x'})])\right]
\end{aligned}
$$

Taking expectations and differentiating,

$$
\begin{aligned}
\frac{\partial}{\partial t}\left(h_1, C_{c\vec{V}_i}(\vec{x},\vec{x'},t)h_2\right) = & \frac{\partial}{\partial t}\mathbf{E}[(h_1, c(\vec{x},t))(h_2, \vec{V}_i(\vec{x'})] \\
& - \mathbf{E}\left[\left(h_1, \frac{\partial}{\partial t}c(\vec{x},t)\right)\left(h_2, \mathbf{E}[\vec{V}_i(\vec{x'}]\right)\right] \\
= & \left(h_1, \left[\mathbf{E}\left[\frac{\partial}{\partial t}c(\vec{x},t)\vec{V}_i(\vec{x'})\right] - \frac{\partial}{\partial t}\mathbf{E}[c(\vec{x},t)]\mathbf{E}[\vec{V}_i(\vec{x'})]\right] h_2\right)
\end{aligned}
$$

Substituting expressions for $\frac{\partial}{\partial t}c(\vec{x},t)$ and $\frac{\partial}{\partial t}\mathbf{E}[c(\vec{x},t)]$ yields

$$
\begin{aligned}
\frac{\partial}{\partial t}\left(h_1, C_{c\vec{V}_i}(\vec{x},\vec{x'},t)h_2\right) = & \left(h_1, \left[\mathbf{E}\left[-\left\{\nabla_{\vec{x}} \cdot c(\vec{x},t)(\mathbf{E}[\vec{V}(\vec{x})] + \vec{V}'(\vec{x}))\right.\right.\right.\right. \\
& \left.\left. - \nabla_{\vec{x}} \cdot (\mathbf{D}\nabla_{\vec{x}} c(\vec{x},t))\right\} \vec{V}_i(\vec{x'})\right] \\
& + \left\{\nabla_{\vec{x}} \cdot (\mathbf{E}[c(\vec{x},t)]\mathbf{E}[\vec{V}(\vec{x})]) - \nabla_{\vec{x}} \cdot (\mathbf{D}\nabla_{\vec{x}} \mathbf{E}[c(\vec{x},t)])\right. \\
& \left.\left.\left. + \nabla_{\vec{x}} \cdot \mathbf{E}[c'(\vec{x},t)\vec{V}'(\vec{x'})]\right\} \mathbf{E}[\vec{V}_i(\vec{x'})]\right] h_2\right)
\end{aligned}
$$

Let $c(\vec{x},t) = \mathbf{E}[c(\vec{x},t)] + c'(\vec{x},t)$ and expand

$$\frac{\partial}{\partial t}\left(h_1, C_{c\vec{V}_i}(\vec{x},\vec{x'},t)h_2\right) = \left(h_1, \left[\mathbf{E}\left[-\left\{\nabla_{\vec{x}}\cdot\mathbf{E}[c(\vec{x},t)]\mathbf{E}[\vec{V}(\vec{x})] + \nabla_{\vec{x}}\cdot c'(\vec{x},t)\mathbf{E}[\vec{V}(\vec{x})]\right.\right.\right.\right.$$

$$+\nabla_{\vec{x}}\cdot\mathbf{E}[c(\vec{x},t)]\vec{V'}(\vec{x}) + \nabla_{\vec{x}}\cdot c'(\vec{x},t)\vec{V'}(\vec{x})$$

$$\left.\left. -\ \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}\mathbf{E}[c(\vec{x},t)]) - \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}c'(\vec{x},t))\right\}\vec{V}_i(\vec{x'})\right]$$

$$+\left\{\nabla_{\vec{x}}\cdot(\mathbf{E}[c(\vec{x},t)]\mathbf{E}[\vec{V}(\vec{x})]) - \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}\mathbf{E}[c(\vec{x},t)])\right.$$

$$\left.\left.\left. +\ \nabla_{\vec{x}}\cdot\mathbf{E}[c'(\vec{x},t)\vec{V'}(\vec{x'})]\right\}\mathbf{E}[\vec{V}_i(\vec{x'})]\right]h_2\right)$$

And, finally, by letting $\vec{V}_i(\vec{x'}) = \mathbf{E}[\vec{V}_i(\vec{x'})] + \vec{V'}_i(\vec{x'})$ and expanding again

$$\frac{\partial}{\partial t}\left(h_1, C_{c\vec{V}_i}(\vec{x},\vec{x'},t)h_2\right) = \left(h_1, \left[\mathbf{E}\left[-\left\{\nabla_{\vec{x}}\cdot\mathbf{E}[c(\vec{x},t)]\mathbf{E}[\vec{V}(\vec{x})]\mathbf{E}[\vec{V}_i(\vec{x'})]\right.\right.\right.\right.$$

$$+\nabla_{\vec{x}}\cdot\mathbf{E}[c(\vec{x},t)]\mathbf{E}[\vec{V}(\vec{x})]\vec{V'}(\vec{x'})$$

$$+\nabla_{\vec{x}}\cdot c'(\vec{x},t)\mathbf{E}[\vec{V}(\vec{x})]\mathbf{E}[\vec{V}_i(\vec{x'})] + \nabla_{\vec{x}}\cdot c'(\vec{x},t)\mathbf{E}[\vec{V}(\vec{x})]\vec{V'}_i(\vec{x'})]$$

$$+\nabla_{\vec{x}}\cdot\mathbf{E}[c(\vec{x},t)]\vec{V'}(\vec{x})\mathbf{E}[\vec{V}_i(\vec{x'})] + \nabla_{\vec{x}}\cdot\mathbf{E}[c(\vec{x},t)]\vec{V'}(\vec{x})\vec{V'}_i(\vec{x'})$$

$$+\nabla_{\vec{x}}\cdot c'(\vec{x},t)\vec{V'}(\vec{x})\mathbf{E}[\vec{V}_i(\vec{x'})] + \nabla_{\vec{x}}\cdot c'(\vec{x},t)\vec{V'}(\vec{x})\vec{V'}_i(\vec{x'})$$

$$-\nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}\mathbf{E}[c(\vec{x},t)]\mathbf{E}[\vec{V}_i(\vec{x'})]) - \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}\mathbf{E}[c(\vec{x},t)]\vec{V'}_i(\vec{x'}))$$

$$\left.\left. -\ \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}c'(\vec{x},t)\mathbf{E}[\vec{V}_i(\vec{x'})]) - \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}c'(\vec{x},t)\vec{V'}_i(\vec{x'})\right\}\right]$$

$$+\left\{\nabla_{\vec{x}}\cdot(\mathbf{E}[c(\vec{x},t)]\mathbf{E}[\vec{V}(\vec{x})]) - \nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}\mathbf{E}[c(\vec{x},t)])\right.$$

$$\left.\left.\left. +\ \nabla_{\vec{x}}\cdot\mathbf{E}[c'(\vec{x},t)\vec{V'}(\vec{x'})]\right\}\mathbf{E}[\vec{V}_i(\vec{x'})]\right]h_2\right)$$

So, by taking expectations, cancelling terms and using the conditions $\mathbf{E}[\vec{V'}] = \mathbf{E}[c'] = 0$, the final equation for the velocity-concentration equation is

$$\begin{aligned}\frac{\partial}{\partial t}\left(h_1, C_{c\vec{V}_i}(\vec{x},\vec{x'},t)h_2\right) &= -\left(h_1, \nabla_{\vec{x}}\cdot\mathbf{E}[\vec{V}(\vec{x})]C_{c\vec{V}_i}(\vec{x},\vec{x'},t)\right.\\ &+\ \nabla_{\vec{x}}\cdot\mathbf{E}[c(\vec{x},t)]C_{\vec{V}_i\vec{V}}(\vec{x},\vec{x'},t)\\ &+\ \nabla_{\vec{x}}\cdot\mathbf{E}[c'(\vec{x},t)\vec{V'}(\vec{x})\vec{V}_i(\vec{x'})]\\ &-\ \left.\nabla_{\vec{x}}\cdot(\mathbf{D}\nabla_{\vec{x}}C_{c\vec{V}_i}(\vec{x},\vec{x'},t))h_2\right)\end{aligned}$$

which agrees with the previously obtained velocity-concentration Equation[7], page 3.

Where real-valued stochastic processes are involved, the derivatives in the previous example are to be interpreted in the mean-squared sense, *i.e.*, if $\xi(t,\omega)$ is a real-valued random function such that for the probability space $(\Omega, \mathcal{F}, P)$

$$\xi : [0,T] \times \Omega \to \Re^1$$

then its derivative with respect to t is given by

$$\begin{aligned}
\frac{d\xi}{dt}(t,\omega) &= \dot{\xi}(t,\omega) = (m^2)\lim_{h\to 0}\frac{\xi(t+h,\omega)-\xi(t,\omega)}{h} \\
&\Rightarrow \quad \lim_{h\to 0}\mathbf{E}\left[\left|\frac{\xi(t+h,\omega)-\xi(t,\omega)}{h}-\dot{\xi}(t,\omega)\right|^2\right]=0 \\
&\Rightarrow \quad \lim_{h\to 0}\int_\Omega\left|\frac{\xi(t+h,\omega)-\xi(t,\omega)}{h}-\dot{\xi}(t,\omega)\right|^2 dP=0
\end{aligned}$$

Linearity of the derivative follows easily from this and the inequality

$$|f+g|^2 \leq 2\left(|f|^2+|g|^2\right)$$

for suppose that the derivatives $\frac{d}{dt}(f+g)$, $\frac{df}{dt}$ and $\frac{dg}{dt}$ exist in the mean-squared sense -

$$\frac{d}{dt}(f+g) = (m^2)\lim_{h\to 0}\frac{(f+g)(t+h,\omega)-(f+g)(t,\omega)}{h} \tag{26}$$

$$\frac{df}{dt} = (m^2)\lim_{h\to 0}\frac{f(t+h,\omega)-f(t,\omega)}{h} \tag{27}$$

$$\frac{dg}{dt} = (m^2)\lim_{h\to 0}\frac{g(t+h,\omega)-g(t,\omega)}{h} \tag{28}$$

Then, in the limit

$$\begin{aligned}
&\lim_{h\to 0}\mathbf{E}\left[\left|\frac{(f+g)(t+h,\omega)-(f+g)(t,\omega)}{h}-\frac{df}{dt}(t,\omega)-\frac{dg}{dt}(t,\omega)\right|^2\right] = \\
&\quad \lim_{h\to 0}\mathbf{E}\left[\left|\left(\frac{f(t+h,\omega)-f(t,\omega)}{h}-\frac{df}{dt}(t,\omega)\right)+\left(\frac{g(t+h,\omega)-g(t,\omega)}{h}-\frac{dg}{dt}(t,\omega)\right)\right|^2\right] \\
&\leq 2\lim_{h\to 0}\left[\mathbf{E}\left[\left|\frac{f(t+h,\omega)-f(t,\omega)}{h}-\frac{df}{dt}(t,\omega)\right|^2\right]+\mathbf{E}\left[\left|\frac{g(t+h,\omega)-g(t,\omega)}{h}-\frac{dg}{dt}(t,\omega)\right|^2\right]\right] \\
&= 0
\end{aligned}$$

from Equation[27] and Equation[28]. Hence, from Equation[26],

$$\frac{d}{dt}(f+g) = \frac{df}{dt}+\frac{dg}{dt} \tag{29}$$

The interchange of the differentiation and expectation operators in the previous example is not obvious and does require justification. The derivative of a stochastic process is the result of a mean squared convergence or a convergence in measure, while the derivative of an expectation is an ordinary derivative. Consequently, if the stochastic process $\xi(t)$ is mean square differentiable, then given the probability space $(\Omega, \mathcal{F}, P)$

$$\lim_{h\to 0}\mathbf{E}\left[\left|\frac{\xi(t+h,\omega)-\xi(t,\omega)}{h}-\dot{\xi}(t,\omega)\right|^2\right]=0$$

Then,

$$\begin{aligned}
\left\{\mathbf{E}\left[\left|\dot{\xi}(t,\omega)-\frac{\xi(t+h,\omega)-\xi(t,\omega)}{h}\right|^{2}\right]\right\}^{\frac{1}{2}} &= \left\{\int_{\Omega}\left|\dot{\xi}(t,\omega)-\frac{\xi(t+h,\omega)-\xi(t,\omega)}{h}\right|^{2}dP\right\}^{\frac{1}{2}} \\
&= \left(\int_{\Omega}\left|\dot{\xi}(t,\omega)-\frac{\xi(t+h,\omega)-\xi(t,\omega)}{h}\right|^{2}dP\right)^{\frac{1}{2}}\left(\int_{\Omega}dP\right)^{\frac{1}{2}} \\
&\geq \int_{\Omega}\left|\dot{\xi}(t,\omega)-\frac{\xi(t+h,\omega)-\xi(t,\omega)}{h}\right|dP \\
&\geq \left|\int_{\Omega}\dot{\xi}(t,\omega)-\frac{\xi(t+h,\omega)-\xi(t,\omega)}{h}dP\right| \\
&= \left|\mathbf{E}[\dot{\xi}(t,\omega)]-\frac{\mathbf{E}[\xi(t+h,\omega)]-\mathbf{E}[\xi(t,\omega)]}{h}\right| \\
&\geq 0
\end{aligned}$$

So, as $h \to 0$ it follows that

$$\mathbf{E}[\dot{\xi}(t,\omega)] = \frac{d}{dt}\mathbf{E}[\xi(t,\omega)]$$

The second example involves measurement uncertainty. This example will shows how the trace term in Equation[18] can be used. Consider

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\vec{V}) - \nabla \cdot (\mathbf{D}\nabla c) = 0 \tag{30}$$

Suppose that there is measurement uncertainty in the laboratory experiment, and that this uncertainty is random. Then, in the laboratory, the experimenters will record the results $\bar{c}$, and the variables u and $\bar{c}$ will be related by

$$\bar{c}(\vec{x},t,\omega) = c(\vec{x},t) + \epsilon(t,\omega) \tag{31}$$

Substituting Equation[31] in Equation[30] yields

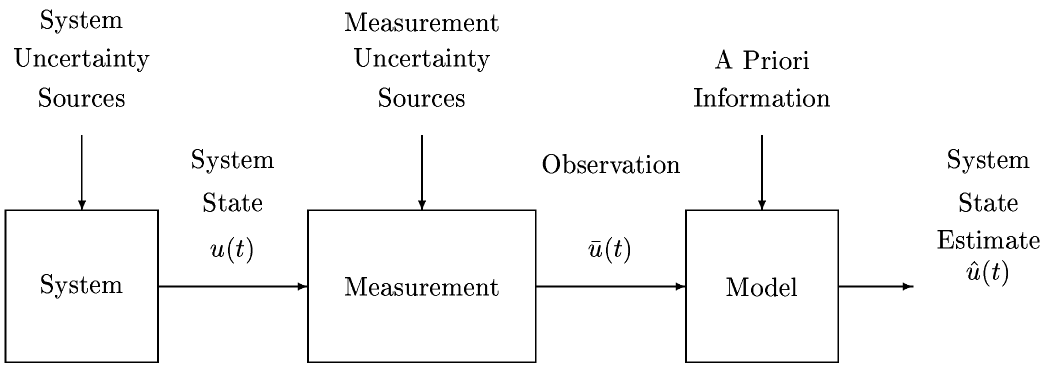
$$\frac{\partial(\bar{c}(\vec{x},t,\omega) - \epsilon(t,\omega))}{\partial t} + \nabla \cdot (\bar{c}(\vec{x},t,\omega)\vec{V}) - \nabla \cdot (\mathbf{D}\nabla\bar{c}(\vec{x},t,\omega) = 0 \tag{32}$$

and, from Equation[29, Equation[32] can be written as

$$\frac{\partial\bar{c}(\vec{x},t,\omega)}{\partial t} + \nabla \cdot (\bar{c}(\vec{x},t,\omega)\vec{V}) - \nabla \cdot (\mathbf{D}\nabla\bar{c}(\vec{x},t,\omega) = \frac{d\epsilon(t,\omega)}{dt}$$

where $\frac{d\epsilon}{dt}$ is a stochastic process. Hence, the introduction of measurement uncertainty is equivalent to applying a stochastic forcing term to the equation.

The situation can be characterized by the following diagram similar to one found in Gelb[45]:

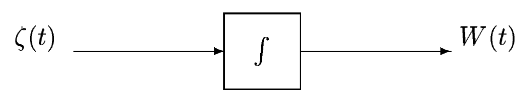


In this diagram, the System Uncertainty Sources are represented by any uncertainty that may exist in the specification of $\mathbf{D}$ and $\vec{V}$, the Measurement Uncertainty Sources are represented by ϵ.

The random forcing term is assumed to be a Gaussian white noise process. This is equivalent to assuming that the process, $\epsilon(t, \omega)$, is a Wiener process which can be defined as the limit of a *random walk*, or as the integral of a Gaussian white noise process with zero mean.

$$W(t) = \int_0^t \zeta(s) ds$$

The following is a block diagram representation of this equation:



$$E[\zeta(t)\zeta(\tau)] = q(t)\delta(t-\tau)$$

The measurement error effect can be illustrated with the following space-time example where the spatial dimension is restricted to be one dimensional: A second feature of the Boulder experiments that must be modeled is the *pulsed input* feature of the experiment. This means that in the tracer experiment, the tracer, benzene, is injected at a rate of 5 ml/min for a period of 4 hours and then the injection pump is turned off. However, samples are taken for a period of 8 hours. This means that at a specified measuring point, the sampling device will see the concentrations of benzene first increase, then level off, and finally decrease to zero.

In the finite element model, this allowed for by imposing a non-zero boundary condition at the origin for a specified number of time steps, and then imposing a zero boundary condition at the origin for the remainder of the time steps of the simulation. The following is a segment of code that performs this task:

```
/************************************************************/
/*     Impose The Left Hand Boundary Condition              */
/************************************************************/
      if (nt <= bctimesteps)
         impose_bndy_cond();
      else {
        lbdy = 0.0;
        impose_bndy_cond();
      }
```

Here, the variable *lbdy* is originally input to the program with a non-zero value. Once the specified number of timesteps for injection of the tracer, *bctimesteps*, has passed, *lbdy* is set to zero and the boundary condition function imposes a zero boundary condition on each succeeding time step.

The two graphs on the next page illustrate the output from the finite element program with a pulsed input. The surface shown in Figure 1 is a space-time representation of the concentration. Figure 2 shows a time-slice of this surface. This curve has the same shape as the actual measurements when they are plotted.

Figure 3 entitled *Comparison Time Profile* shows the Pulsed Input Time Profile with and without the effects of a random forcing term (measurement uncertainty). The dotted line represents the time profile without measurement uncertainty, and the solid line shows the time profile with measurement uncertainty taken into consideration.

Returning to the equation

$$\frac{\partial \bar{c}(\vec{x},t,\omega)}{\partial t} + \nabla \cdot (\bar{c}(\vec{x},t,\omega)\vec{V}) - \nabla \cdot (\mathbf{D}\nabla \bar{c}(\vec{x},t,\omega) = \frac{d\epsilon(t,\omega)}{dt}$$

For the sake of simplicity, assume that the parameters $\mathbf{D}$ and $\vec{V}$ are deterministic. This means that there will be no need of a velocity-concentration covariance equation as in the previous example. The equation for the expected value of the concentration takes the form

$$\frac{\partial \mathbf{E}[\bar{c}(\vec{x},t)]}{\partial t} + \nabla \cdot (\mathbf{E}[\bar{c}(\vec{x},t)]\vec{V}(\vec{x})) - \nabla \cdot (\mathbf{D}\nabla \mathbf{E}[\bar{c}(\vec{x},t)]) = 0$$

For the equation of the concentration covariance, let $\vec{x}$ and $\vec{x'}$ be two different coordinate systems, then from Equation[18], page 22,

$$\begin{aligned}
\frac{\partial}{\partial t}(h_1, \bar{c}(\vec{x},t))(h_2, \bar{c}(\vec{x'},t)) &= -\Big[(h_1, \bar{c}(\vec{x},t))(h_2, A_{\vec{x'}}\bar{c}(\vec{x'},t)) \\
&+ (h_1, \bar{c}(\vec{x'},t)(h_2, A_{\vec{x}}\bar{c}(\vec{x},t))\Big] \\
&+ \frac{1}{2} tr\left[(h_2 \circ h_1) \oplus (h_1 \circ h_2) Q(t)\right]
\end{aligned}$$

where $\Gamma = I$. And, by proceeding as in the previous example,

$$\begin{aligned}
\frac{\partial}{\partial t}(h_1, C_{\bar{c}\bar{c}}(\vec{x},\vec{x'},t)h_2) &= -\Big(h_1, \Big[\nabla_{\vec{x}} \cdot \mathbf{E}[\vec{V}(\vec{x})]C_{\bar{c}\bar{c}}(\vec{x},\vec{x'},t) \\
&- \nabla_{\vec{x}} \cdot (\mathbf{D}\nabla_{\vec{x}} C_{\bar{c}\bar{c}}(\vec{x},\vec{x'},t) + \nabla_{\vec{x'}} \cdot \mathbf{E}[\vec{V}(\vec{x'})C_{\bar{c}\bar{c}}(\vec{x'},\vec{x},t)] \\
&- \nabla_{\vec{x'}} \cdot (\mathbf{D}\nabla_{\vec{x'}} C_{\bar{c}\bar{c}}(\vec{x'},\vec{x},t))\Big] h_2\Big) \\
&+ \frac{1}{2} tr\left[(h_2 \circ h_1) \oplus (h_1 \circ h_2) Q(t)\right]
\end{aligned}$$

Finally, substituting for the tr term from Equation[14], page 14, it follows that

$$\begin{aligned}
\frac{\partial}{\partial t}(h_1, C_{\bar{c}\bar{c}}(\vec{x},\vec{x'},t)h_2) &= -\Big(h_1, \Big[\nabla_{\vec{x}} \cdot \mathbf{E}[\vec{V}(\vec{x})]C_{\bar{c}\bar{c}}(\vec{x},\vec{x'},t) \\
&- \nabla_{\vec{x}} \cdot (\mathbf{D}\nabla_{\vec{x}} C_{\bar{c}\bar{c}}(\vec{x},\vec{x'},t) + \nabla_{\vec{x'}} \cdot \mathbf{E}[\vec{V}(\vec{x'})C_{\bar{c}\bar{c}}(\vec{x'},\vec{x},t)]
\end{aligned}$$

Figure 1 - 1D Pulsed Input Over Time

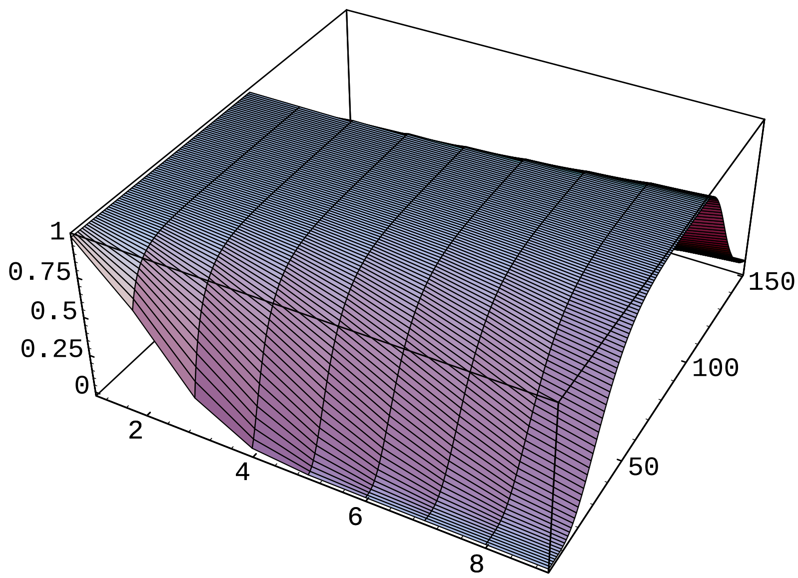


Figure 2 - Pulsed Input Time Slice

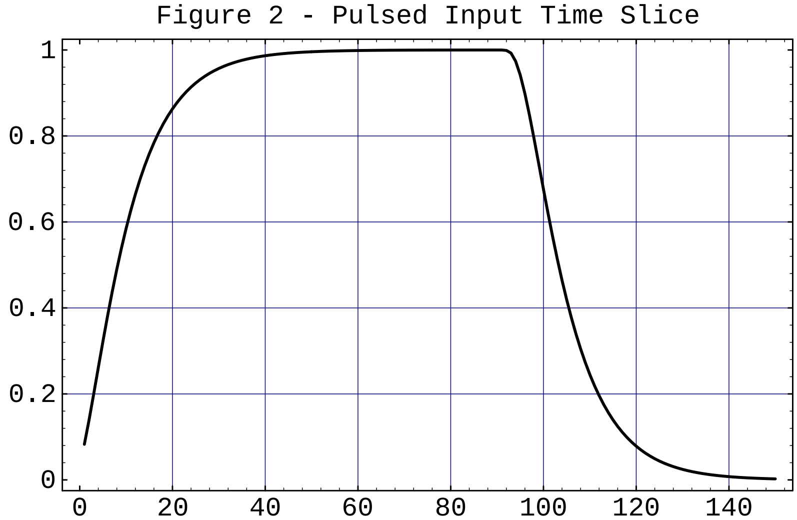
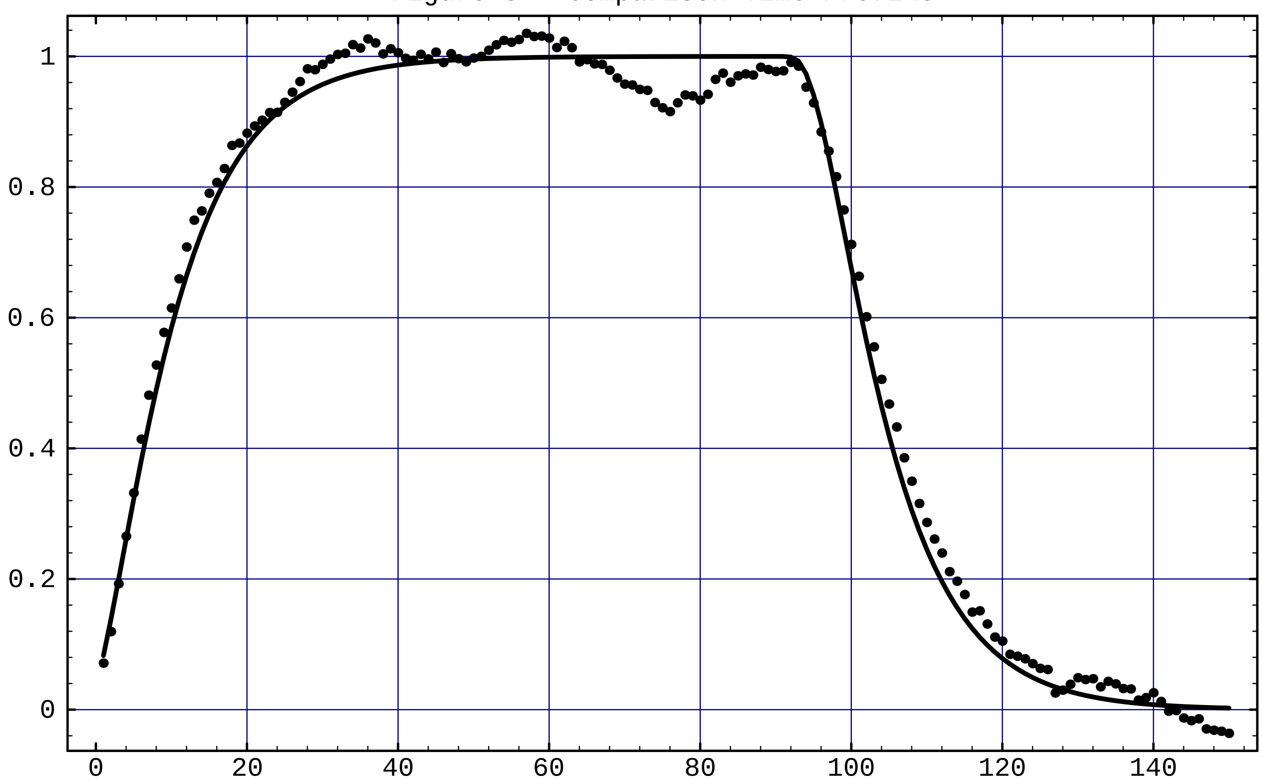


Figure 3 - Comparison Time Profile



$$- \quad \nabla_{\vec{x'}} \cdot (\mathbf{D}\nabla_{\vec{x'}} C_{\bar{c}\bar{c}}(\vec{x'}, \vec{x}, t)) - Q\Big] h_2\Big)$$

4 Summary

Because of the uncertainties involved in specifying the physical characteristics of the porous medium, the concentration of a solute at a given point in time is a random variable, and over a period of time it is a stochastic process. Consequently, in order to more accurately characterize the distribution of the solute concentration, higher order statistical moments such as the variance need to be estimated also. In theory, the more moments that can be predicted, the better this characterization will be. But, in practice, it is usually a difficult problem just to obtain information on the variance or covariance of variables in the system. A much referenced paper in this area is the Graham and McGlaughlin[50] paper which specifies a set of three equations that are to be solved for the mean concentration, the velocity-concentration covariance and the concentration covariance. These equations were presented in Section 2.0 for the purpose of comparison with mean and covariance equations derived from the Itô method.

Randomness can enter the boundary value problem in many different ways. Equation[12], page 6, is a statement of the stochastic boundary value problem, and the discussion following that equation specifies the various ways in which randomness can enter the picture. Existence theory for the stochastic boundary value problem was covered in Section 3.3 and found to be not unlike the nonstochastic case.

Stochastic integration is addressed in Section 3.4 from the more general perspective of a *martingale*. The Itô integral then follows from this more general definition as a special case. The use of the Itô integral requires that the rules of calculus have to be modified. The most important new rule is that of Itô's lemma. It is a change of variable formula or a stochastic calculus chain-rule. It can also be extended to martingale type processes, Karatzas[59]. Curtain and Falb[26] have extended Itô's lemma to infinite dimensional Hilbert spaces. It is this form that is used to derive weak forms of the moment equations in Section 3.8. For the purpose of illustrating this theory, the key equation is Equation[18], page 22, which is applied to two examples. The first example uses this theory to derive mean and covariance equations that in the weak form are identical to those used by Graham and McLaughlin[50]. The second example is cast in terms of accounting for the effects of measurement error that is assumed to enter the experiment as a random perturbation that takes the form of a Wiener process.

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