4.STOCHASTIC THEORY OF UNSATURATED FLOW IN TWO DIMENSIONS

4.1 Mathematical Problem Formulation

Flow in two-dimensional porous media under variably saturated conditions is generally modeled by Richards equation (Hillel, 1980):

$$\frac{\partial}{\partial x_i}\left[K_i(h)\frac{\partial(x_2+h)}{\partial x_i}\right] = C(h)\frac{\partial h}{\partial t} \qquad i=1,2 \qquad \textbf{(4-1)}a$$

where x_1 and x_2 are the horizontal and vertical coordinates, respectively. Note that the denoting of the vertical direction as x_2 (rather than x_1) is unusual (see Yeh, 1985a,b), but is chosen here for consistency with the notation for the numerical model (chapter 5). For the clarity in subsequent chapters, the subscripts x and z are used interchangeably with the subscripts 1 and 2, where appropriate. x_2 is positive upward, h is the matric potential (negative for unsaturated condition). $K_i(h)$, the principal unsaturated hydraulic conductivity, and the moisture capacity term, $C(h)=d\theta/dh$, are functions of h. For simplicity of notation and without loss of generality, it is assumed that the principal axes of anisotropy in the hydraulic conductivity coincide with the principal coordinate axes.

Under steady-state conditions the right-hand side of (2) vanishes and the solution becomes independent of the water retention function $\theta(h)$:

$$\frac{\partial}{\partial x_i}\left[K_i(h)\frac{\partial(x_2+h)}{\partial x_i}\right] = 0 \qquad i=1,2 \qquad \textbf{(4-1)}b$$

Like the groundwater flow equation, Richards equation is based on the principles of Darcy's law (conservation of momentum):

$$q_i = -K_i(h)\frac{\partial(h + x_2)}{\partial x_2} \qquad i=1,2 \tag{4-2}$$

and mass continuity (conservation of mass) :

$$-\nabla \mathbf{q} = \frac{\partial m_w}{\partial t} = C(h)\frac{\partial h}{\partial t} \tag{4-3}$$

q_i is the flux per cross-sectional area $A_i \perp x_i$, and $\partial m_w/\partial t$ is the change of the total mass of water per unit time. Unlike the parameters in the saturated flow equation, the parameters in Richards equation are functions of the matric potential h and hence equations (3-1a) and (3-1b) are nonlinear equations. Parametric relationships must be constructed to relate the unsaturated hydraulic conductivity K, the moisture content θ, and the moisture capacity function C to the matric potential (head) h. Since the moisture capacity function C(h) is defined in terms of θ and h, two functions $K_i(h)$ and $\theta(h)$ are sufficient to complete the transient equation (3-1a). A single function $K_i(h)$ suffices to complete the steady-state equation (3-1b).

Water retention $\theta(h)$ and saturated hydraulic conductivity K_s are commonly measured from soil samples. The measured $\theta(h)$ are used to find the parameters of a theoretical function such that the function will best fit the empirical data. The following class of functions has become particularly useful in describing actual field data (VanGenuchten, 1980):

$$\Theta = \left[\frac{1}{1+(|\alpha h|)^n}\right]^m \qquad m=1-1/n \tag{4-4}$$

where

$$\Theta = \frac{\theta-\theta_r}{\theta_s-\theta_r} \tag{4-5}$$

θ_s is the moisture content at saturation and θ_r is the residual moisture content. m is a fitting parameter related to the tortuosity of the flow path and the correlation between pores. α is a parameter mainly associated with the pore size distribution.

Unlike the water retention relationship or the saturated hydraulic conductivity, the

unsaturated hydraulic conductivity K(h) is much more difficult to measure both in the field and in the laboratory. Since K(h) depends on similar porous medium properties as $\theta(h)$, several models have been developed to determine K(h) as a function of the known water retention relationship. Mualem (1976) suggested the relationship:

$$K(\Theta)=K_s \sqrt{\Theta} \left[\int_0^{\Theta} \frac{1}{h(x)} dx \Big/ \int_0^{1} \frac{1}{h(x)} dx \right]^2 \qquad \textbf{(4-6)}$$

From this and (4-4) VanGenuchten (1980) derived the following K(h) model:

$$K(h) = K_s \frac{[1-(|\alpha h|)^{n-1} [1+(|\alpha h|)^n]^{-m}]^2}{[1+(|\alpha h|)^n]^{\frac{m}{2}}} \qquad (m=1-1/n) \qquad \textbf{(4-7)}$$

Equations (4-4) an (4-7) are commonly known as the VanGenuchten model and have been used to describe a number of scientific field sites related to the study of soil heterogeneity (Anderson and Cassel, 1986; Field et al., 1984; Hopmans and Stricker, 1989; Wierenga et al., 1989, 1991). While the VanGenuchten model has provided the flexibility needed to describe many field soils, its functional form does not lend itself to the analytical study of soil moisture movement. Analytical solutions to Richards equation (4-1) can be derived only with simpler models. The exponential model first suggested by Gardner (1958) provides a powerful class of K(h) functions:

$$K(h) = K_s \exp(\alpha h) \qquad \textbf{(4-8)}$$

Again, α is related to the pore-size distribution and will in the remainder of the text be referred to as the pore-size distribution parameter. In the Gardner model K_s is related to, but need not be taken as, the saturated hydraulic conductivity. This should be kept in mind, as K_s is simply referred to as "saturated hydraulic conductivity" throughout this text.

Russo (1988) developed the following $\theta(h)$ model that is consistent with Gardner's exponential model for K(h) (4-8) and with Mualem's pore-size distribution model (4-8):

$$\theta = \theta_r + (\theta_s - \theta_r)[e^{-0.5\alpha|h|}(1 + 0.5\alpha|h|)]^{2/(m+2)} \quad \textbf{(4-9)}$$

Equations (4-8) and (4-9) are sometimes referred to as the Gardner-Russo model (Russo, 1988).

In the stochastic analysis of unsaturated flow and transport in heterogeneous soils, $K_s(\mathbf{x})$, $\alpha(\mathbf{x})$, $m(\mathbf{x})$, $\theta_s(\mathbf{x})$, and $\theta_r(\mathbf{x})$ become random field variables (RFVs, see chapter 2.5.1). The RFVs are defined by their probability distribution functions. Field studies have shown that the saturated hydraulic conductivity K_s, the pore-size distribution parameter α, and the tortuosity factor m are lognormally distributed (White and Sully, 1992). Little is known about the variability of θ_s and θ_r and the sensitivity of the head and flux solutions to the variability of the parameters defining the water retention functions (4-4) and (4-9). Analytical models commonly neglect the spatial variability in θ or state their results in terms of the flux rather than in terms of pore-velocity (Mantoglou et al., 1987a,b,c; Russo, 1993a; Yeh et al., 1985a,b). For the sake of clarity and since it is not the purpose of this study to investigate the impact of spatially variable θ on the transport behavior of solutes in unsaturated soils, the variability in θ_s, θ_r, m, α, and h in (4-4) and (4-9) will henceforth be ignored. A constant water content θ is assumed throughout the domain. Furthermore, K_s and therefore K(h) are assumed to be locally isotropic i.e., $K_1(\mathbf{x},h) = K_2(\mathbf{x},h)$. In the remainder of this work, K_s and α are the only independent parameters that are assumed spatially variable in the governing equations (4-1) and (4-2) with (4-8) and (4-9) being the constitutive equations.

The numerical steady-state analysis of flow and transport in this study is based on the use of Gardner's exponential K(h) function (4-8), since this K(h) model also allows the derivation of approximate (1st order) analytical solutions. The practicality of using Gardner's K(h) model may be questioned (White and Sully, 1992). But this study is geared towards investigating rather fundamental problems in the numerical stochastic treatment of unsaturated flow and transport. It is justified to confine the numerical modeling to some of the constraints of analytical tools since the theoretical analysis of steady-state unsaturated flow and transport is an important part of this study:

- approximate analytical solutions allow a preliminary evaluation of the physical importance of various parameters to the stochastic head and flux solutions (this chapter);
- approximate analytical solutions are used as initial solutions to the numerical solver to improve the CPU-efficiency of the Monte Carlo analysis by up to two orders of magnitude (see chapter 7);
- analytical solutions serve to validate the numerical models within a range of variability for which analytical solutions are known to be rather accurate (see chapter 6, 8, and 9);
- the range of validity of the approximate analytical solutions is investigated empirically by comparison to numerical solutions for highly heterogeneous soils (see chapter 6, 8, and 9);

Yeh et al. (1985a,b,c) presented a thorough analysis of one- and three-dimensional steady-state unsaturated flow in heterogeneous soils based on Gardner's K(h) model with constant α and with normally distributed α. The following will, for the first time, give a thorough analysis of two-dimensional flow in heterogeneous soils under the more justifiable assumption that α is a lognormally distributed field parameter. In addition spectral analysis will be applied to determine the first and second moments of the unsaturated hydraulic conductivity and of the velocity components. The analytical extension of these results to three dimensions as in Yeh et al. (1985a,b) is straightforward.

4.2 First-Order Perturbation Analysis of the Governing Stochastic Equation

This analysis is based on a first-order perturbation approach similar to the work by Bakr et al. (1978), Gelhar and Axness (1983), and Yeh et al. (1985a,b). Equation (4-1b) can be rewritten as

$$\frac{\partial^2 h}{\partial x_i} + \frac{\partial \log K(h)}{\partial x_i}\frac{\partial h}{\partial x_i} + \frac{\partial \log K(h)}{\partial x_1} = 0 \qquad \textbf{(4-10)}$$

where i=1, 2. Throughout the dissertation, the notation 'log' refers to the natural logarithm (unless otherwise noted). The following perturbation notation is used for the random variables $\log K_s$ $\log\alpha$, and h:

$$\begin{aligned} \log K_s(\mathbf{x}) &= f = F(\mathbf{x}) + f'(\mathbf{x}) \\ \log\alpha(\mathbf{x}) &= a = A(\mathbf{x}) + a'(\mathbf{x}) \\ h(\mathbf{x}) &= H(\mathbf{x}) + h'(\mathbf{x}) \end{aligned} \qquad \textbf{(4-11)}$$

where $F(\mathbf{x})$, $A(\mathbf{x})$, and $H(\mathbf{x})$ are the expected values of $\log K_s(\mathbf{x})$, $\log\alpha(\mathbf{x})$, and $h(\mathbf{x})$, respectively, and $f'(\mathbf{x})$, $a'(\mathbf{x})$, and $h'(\mathbf{x})$ are zero-mean, second order stationary perturbations at location $\mathbf{x}$. For the sake of brevity, the explicit dependency of the RFVs, their mean, and their perturbation on the location $\mathbf{x}$ will be omitted from now on.

In general H is not uniform in space, but the gradient of H, $J_i=\partial H/\partial x_i$, is assumed to be independent of location. The unsaturated hydraulic conductivity is then given by

$$\begin{aligned} \log K(h) &= \log K_s + \alpha h \\ &= F + f' + (H + h')\exp(A + a') \end{aligned} \qquad \textbf{(4-12)}$$

Writing $\exp(A+a') = \exp(A)\exp(a')$ and expanding the exponential perturbation term in a Taylor series gives:

$$\exp(a') = 1 + (a') + \frac{(a')^2}{2!} + \ldots \qquad \textbf{(4-13)}$$

Writing the geometric mean of α as $\Gamma=\exp(A)$ and truncating the Taylor series to first order, the unsaturated hydraulic conductivity can also be approximated by a lognormally distributed random variable:

$$\log K_s = Y + y' = F + f' + (1+a')\,\Gamma\,(H+h') \qquad \textbf{(4-14)}$$

where Y is the mean of logK(h) and y' is a zero-mean, second order stationary random perturbation. Expanding the product terms and again neglecting second-order terms the first-order perturbation approximation of the unsaturated hydraulic conductivity is obtained:

$$Y + y' = F + f' + H\Gamma + \Gamma h' + H\Gamma a' \qquad \textbf{(4-15)}$$

Using (4-15) in (4-10) the stochastic form of Richards equation becomes:

$$\frac{\partial^2(H+h')}{\partial x_i^2} + \frac{\partial}{\partial x_i}\left[(F+f'+H\Gamma+\Gamma h'+H\Gamma a')\frac{\partial(H+h')}{\partial x_i}\right] + \frac{\partial}{\partial x_2}(F+f'+H\Gamma+\Gamma h'+H\Gamma a') = 0$$

Expanding the product terms, neglecting second and higher order terms, and noticing that the derivatives of the mean of stationary random field variables are zero, the first order stochastic Richards equation is:

$$\frac{\partial^2 h'}{\partial x_i} + J_i\frac{\partial f'}{\partial x_i} + \Gamma J_i^2 + 2\Gamma J_i\frac{\partial h'}{\partial x_i} + \Gamma J_i^2 a' + \Gamma H J_i\frac{\partial a'}{\partial x_i} + \frac{\partial f'}{\partial x_2} + \Gamma J_2 + \Gamma\frac{\partial h'}{\partial x_2} + \Gamma a' J_2 + \Gamma H\frac{\partial a'}{\partial x_2} = 0 \qquad \textbf{(4-17)}$$

Taking the expected values, the mean Richards equation is:

$$\Gamma J_i^2 + \Gamma J_2 = 0 \qquad \textbf{(4-18)}$$

Subtracting the mean equation from the stochastic equation, the governing perturbation equation becomes:

$$\frac{\partial^2 h'}{\partial x_i} + J_i\frac{\partial f'}{\partial x_i} + 2\Gamma J_i\frac{\partial h'}{\partial x_i} + \Gamma J_i^2 a' + \Gamma H J_i\frac{\partial a'}{\partial x_i} + \frac{\partial f'}{\partial x_2} + \Gamma\frac{\partial h'}{\partial x_2} + \Gamma a' J_2 + \Gamma H\frac{\partial a'}{\partial x_2} = 0 \qquad \textbf{(4-19)}$$

This study is particularly concerned with cases involving gravity drainage conditions i.e., the average gradient of the total potential $\Phi=(h+x_2)$ is unity and the average gradient of h is zero in all directions: $J_i = 0$. Although the entire following analysis can be carried out for any constant mean gradients J_i, only the solutions for zero mean head gradient will be given. In that case H is uniform in space i.e., independent of location. The governing perturbation equation then simplifies to:

$$\frac{\partial^2 h'}{\partial x_i} + \frac{\partial f'}{\partial x_2} + \Gamma\frac{\partial h'}{\partial x_2} + \Gamma H\frac{\partial a'}{\partial x_2} = 0 \qquad \textbf{(4-20)}$$

Note that this is a linear equation. The linearization has been achieved by dropping the higher order perturbation products.

The head covariance function, the cross-covariance function between f' and h', and the covariance and cross-covariance functions of flux related RFVs are obtained from a spectral analysis of the respective second order stationary random processes. Continuous parameter stationary processes in infinite domains can be represented by Fourier-Stieltjes integrals (see chapter 2):

$$a'(\mathbf{x}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}}\, dZ_{a'}(\mathbf{k})$$

$$f'(\mathbf{x}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}}\, dZ_{f'}(\mathbf{k}) \qquad \textbf{(4-21)}$$

$$h'(\mathbf{x}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}}\, dZ_{h'}(\mathbf{k})$$

$dZ_p(\mathbf{k})$ are orthogonal complex stochastic processes, p = f', a', or h', where:

$$\langle dZ_p(k)\rangle = 0$$

$$\langle dZ_p^*(k_m)\, dZ_p(k_n)\rangle = 0 \qquad m \neq n \qquad \textbf{(4-22)}$$

$$\langle dZ_p^*(k_m)\, dZ_p(k_n)\rangle = S_{pp}(k)\,dk \qquad m = n$$

where * indicates complex conjugate. In other words, the process $dZ_p(\mathbf{k})$ is a zero-mean univariate Gaussian random variable. Any $dZ_p(\mathbf{k}_m)$ is statistically independent of $dZ_p(\mathbf{k}_n)$ for $m \neq n$ and has a variance $S_{pp}(\mathbf{k})\, d\mathbf{k}$. $S_{pp}(\mathbf{k})$ is the Fourier transform of the covariance functions for the spatial random processes $X_p(\mathbf{x}) = f'(\mathbf{x})$, $a'(\mathbf{x})$, or $h'(\mathbf{x})$. Similarly the cross-spectral density $S_{pq}(\mathbf{k}) = \langle dZ^*_p(\mathbf{k})\, dZ_q(\mathbf{k})\rangle$ is the Fourier transform of the cross-covariance function between the processes p and q (p, q = f', a', or h'). The general relationship between the (cross-) covariance and the (cross-) spectral density is defined by (3-4):

$$C_{pq}(\xi) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\xi}\, S_{pq}(\mathbf{k})\, d\mathbf{k} \qquad \textbf{(4-23)}$$

Note that $C_{pq}(\xi) = C_{pq}(\mathbf{x}, \mathbf{x}+\xi)$. This can be shown by using the definition for $S_{pq}(\mathbf{k}) = \langle dZ^*_p(\mathbf{k})\, dZ_q(\mathbf{k})\rangle$ and expanding the complex exponential in (4-23) to $\exp(i\mathbf{k}(\mathbf{x}-\mathbf{x}+\xi))$, which leads to

$$C_{pq}(\xi) = < \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i\mathbf{k}\cdot\mathbf{x}}\, dZ_p^*(\mathbf{k}) \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i\mathbf{k}(\mathbf{x}+\xi)}\, dZ_q(\mathbf{k}) >$$

$$= < X_p^*(\mathbf{x})\, X_q(\mathbf{x}+\xi) > \qquad \textbf{(4-24)}$$

$$= < X_p(\mathbf{x})\, X_q(\mathbf{x}+\xi) >$$

Using (4-22) and (4-23), (cross-) covariance functions of dependent variables are obtained from their spectral representations $dZ_p(\mathbf{k})$, which in turn are functions of the independent random fields $dZ_{f'}(\mathbf{k})$ and $dZ_{a'}(\mathbf{k})$.

Using the spectral representation of the random variables f'(**x**), a'(**x**), and h'(**x**) (4-21) to expand the governing first order perturbation equation (4-20), and taking the derivatives with respect to the spatial coordinates, the partial differential equation becomes an integral equation:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i\mathbf{k}\cdot\mathbf{x}}[(-(k_1^2 + k_2^2)+ik_2\Gamma)dZ_{h'} + (ik_2)dZ_{f'} + ik_2H\Gamma dZ_{a'}] = 0 \qquad \textbf{(4-25)}$$

[As with the spatial RFVs and for the sake of clarity, the dependency of dZ_p on **k** is implicitly assumed and not denoted explicitly.] Because of the uniqueness of the spectral representation theorem, the integral (4-25) is only zero, if the expression in square brackets becomes zero. The solution to (4-25) is an explicit closed form expression for the relationship between the Fourier amplitudes of the independent RFVs a', f', and the dependent RFV h':

$$dZ_{h'} = \frac{ik_2(dZ_{f'} + H\Gamma dZ_{a'})}{(k_1^2 + k_2^2 - i\Gamma k_2)} \qquad \textbf{(4-26)}$$

The reader is reminded that this is an exact solution to the first order perturbation equation governing steady-state unsaturated flow in an infinite, vertically two-dimensional domain under gravity drainage. It is also an exact, but trivial solution to the fully perturbed Richards equation with arbitrary boundary conditions at an infinite distance in the limit as $\sigma^2_{f'}$->0 and $\sigma^2_{a'}$->0. For $\sigma^2_{f'}$<<1 and $\sigma^2_{a'}$<<1 the above solution may be taken as a valid approximation of the

solution to the nonlinear Richards equation, since higher order perturbation products that were disregarded during the derivation of (4-26) are indeed negligibly small.

4.3 Moment Analysis of Unsaturated Flow

4.3.1 Head

The previous section derives an explicit spectral head solution for the first order perturbation flow equation. The mean head H is assumed to be a known constant parameter (gravity drainage). The variance and covariance of the head are obtained from an inverse Fourier transform of the spectral density, which can be computed numerically (see section 4.4). The spectral density is related to the spectral representation through (4-22c). Hence the remaining step in the derivation of the head variance-covariance function is to take the expected value of the products of $dZ_{h'}$ and its conjugate complex $dZ_{h'}$*:

$$S_{hh} = \langle dZ_h^*, dZ_h \rangle = \frac{k_2^2 (S_{ff} + 2H\Gamma S_{fa} + H^2\Gamma^2 S_{aa})}{(k_1^2+k_2^2)^2 + \Gamma^2 k_2^2} \qquad \textbf{(4-27)}$$

Although not explicitly stated (for reasons of brevity) S_{hh} and all following spectral density functions S_{pq} are functions of **k**. Also for simplicity of notation, the ' are dropped from the subscripts to the spectral density S and the covariance function C. S_{ff} and S_{aa} are the Fourier transforms of the covariance functions C_{ff} and $C_{aa,}$ respectively, and can be obtained analytically for some covariance functions (Bakr, 1978; Mizell, 1981). The cross-spectral density S_{fa} depends on the desired cross-correlation between f'(**x**) and a'(**x**+ξ). A more general treatise on generating cross-correlated random fields can be found in Robin et al. (1993).

When $C_{aa}/\sigma^2_a = C_{ff}/\sigma^2_f$ i.e., the correlation functions of a' and f' are identical, a' and f' are related through the following relationship:

$$a' = \zeta \left(\rho f' + \sqrt{1-\rho^2}\, w' \right) \tag{4-28}$$

where $\zeta = \sigma_a/\sigma_f$, ρ is the local correlation between f'(**x**) and a'(**x**), and w'(**x**) is a random process uncorrelated to f'(**x**) but with the same covariance function. Then it is easily seen by inspection that

$$dZ_{a'} = \zeta \left(\rho dZ_{f'} + \sqrt{1-\rho^2} dZ_{w'} \right) \tag{4-29}$$

From this it follows immediately that

$$\begin{aligned} S_{aa} &= \zeta^2 S_{ff} \\ S_{af} &= \zeta \rho S_{ff} \end{aligned} \tag{4-30}$$

and the head spectral density function simplifies to:

$$S_{hh} = \frac{k_2^2}{(k_1^2 + k_2^2)^2 + \Gamma^2 k_2^2} \left(1 + 2\rho\zeta H\Gamma + (\zeta H\Gamma)^2\right) S_{ff} \tag{4-31}$$

The cross-spectral densities between f' and h' and between a' and h' are:

$$S_{fh} = < dZ_{f'}^*, dZ_{h'} > = (-\Gamma k_2^2 + i\, k_2 (k_1^2 + k_2^2)) \frac{(S_{ff} + H\Gamma S_{fa})}{(k_1^2 + k_2^2)^2 + \Gamma^2 k_2^2)} \tag{4-32}$$

$$S_{ah} = < dZ_{a'}^*, dZ_{h'} > = (-\Gamma k_2^2 + i\, k_2 (k_1^2 + k_2^2)) \frac{(S_{af} + H\Gamma S_{aa})}{(k1^2 + k_2^2)^2 + \Gamma^2 k_2^2)} \tag{4-33}$$

If the correlation functions of a' and f' are identical, definition (4-29) is used to replace S_{aa} and $S_{af} = S_{fa}$ in (4-32) and (4-33), and to write S_{ah}:

$$S_{ah} = \frac{\zeta\rho + \zeta^2 H\Gamma}{1 + \zeta\rho H\Gamma} S_{fh} \tag{4-34}$$

Note that $S_{fh}^* = S_{hf}$, and $S_{ah}^* = S_{ha}$ which can be seen by inspection of (4-24). Since the cross-spectral densities S_{fh} and S_{ah} are even in the real parts, but odd in the quadrature spectra with

respect to k_2, the resulting cross-covariances are symmetric in the direction normal to the mean flow x_1, but asymmetric in the direction parallel to mean flow x_2 i.e., $C_{fh} \neq C_{hf}$ and $C_{ah} \neq C_{ha}$!

All the necessary moments to determine the parameters of the multivariate Gaussian probability density function of the matric potential h are now defined. These analytical relationships are strictly valid only for small perturbations with $\sigma^2_{f'} << 1$ and $\sigma^2_{a'} << 1$.

4.3.2 Unsaturated Hydraulic Conductivity

Recall the first order perturbation approximation of the logarithms of unsaturated hydraulic conductivity given in (4-15). Taking the expectation of (4-15) the equation for the 1st order mean unsaturated hydraulic conductivity Y is:

$$Y = F + H\Gamma \tag{4-35}$$

Subtracting (4-35) from (4-15), the perturbation y' of the unsaturated hydraulic conductivity becomes:

$$y' = f + \Gamma h' + H\Gamma a' \tag{4-36}$$

Again the spectral representations of f', a', and h' (4-21) are used to obtain a spectral

$$dZ_{y'} = dZ_{f'} + \Gamma dZ_{h'} + H\Gamma dZ_{a'} \tag{4-37}$$

representation of y':

Then the spectral density of y', S_{yy}, is the expectation of the product of $dZ_{y'}$ with its complex conjugate:

$$\begin{aligned} S_{yy} &= S_{ff} + \Gamma^2 S_{hh} + (H\Gamma)^2 S_{aa} + 2H\Gamma S_{fa} \\ &+ \Gamma(S_{fh} + S^*_{fh}) + \Gamma H\Gamma(S_{ah} + S^*_{ah}) \end{aligned} \tag{4-38}$$

where * indicates complex conjugate. When $C_{aa} = \zeta^2 C_{ff}$ relationships (4-29) and (4-30) are applied to obtain the spectral density S_{yy} in terms of S_{ff}:

$$S_{yy} = \left[1 + \frac{-k_2^2\Gamma^2}{(k_1^2 + k_2^2)^2 + \Gamma^2 k_2^2}\right](1 + 2\rho\zeta H\Gamma + (\zeta H\Gamma)^2)\, S_{ff} \qquad \textbf{(4-39)}$$

Similarly, the cross-spectral density S_f is

$$S_{fy} = S_{ff} + \Gamma S_{fh} + H\Gamma S_{fa} \qquad \textbf{(4-40)}$$

As with the cross-spectral densities S_{fh} and S_{ah} , S_f and hence C_f are nonsymmetric functions and care must be taken to apply the correct definition of the lag (4-24), when using these cross-covariance functions.

4.3.3 Pore Velocity

Pore velocity is defined by dividing the Darcy flux (4-2) with the soil water content θ:

$$v_n = \frac{-K(h)}{\theta}\frac{\partial(h + x_2)}{\partial x_n} \qquad \textbf{(4-41)}$$

Using the first order approximation of K(h) given in (4-15), assuming that the mean head is the same everywhere (gravity drainage), and expanding esp(y') into a first order Taylor series similar to that of esp(a') in (4-13), the velocity components are approximated by:

$$v_1 = \frac{-K_m}{\theta}(1 + y')\, j_1'$$
$$v_2 = \frac{-K_m}{\theta}(1 + y')(1 + j_2') \qquad \textbf{(4-42)}$$

where K_m = esp(Y) and $j_n' = \partial h'/\partial x_n'$. The expected value of (4-42) gives the stationary first order mean velocity components:

$$V_1 = \langle v_1 \rangle = 0$$
$$V_2 = \langle v_2 \rangle = \frac{-K_m}{\theta} \qquad \textbf{(4-43)}$$

Subtracting the expressions in (4-43) from the stochastic representation of the velocity v in (4-42), first order, zero mean velocity perturbations are obtained:

$$v_1' = \frac{-K_m}{\theta} j_1'$$
$$v_2' = \frac{-K_m}{\theta}(y' + j_2') \qquad \textbf{(4-44)}$$

By simple inspection, and noting that $dZ_{j'n} = ik_n dZ_{h'}$ it is seen that the corresponding spectral representations of the velocity components are

$$dZ_{v_1'} = \frac{-K_m}{\theta}(ik_2 dZ_{h'})$$
$$dZ_{v_2'} = \frac{-K_m}{\theta}(dZ_{f'} + H\Gamma dZ_{a'} + (\Gamma + ik_1)dZ_{h'}) \qquad \textbf{(4-45)}$$

Recall that $S_{v1.v1} = \langle dZ_{v1}^* \, dZ_{v1} \rangle$ and $S_{v2.v2} = \langle dZ_{v2}^* \, dZ_{v2} \rangle$. Then the Fourier transforms of the velocity covariance functions are:

$$S_{v_1v_1} = \frac{K_m^2}{\theta^2} k_1^2 S_{hh}$$

$$S_{v_2v_2} = \frac{K_m^2}{\theta^2} [S_{ff} + (H\Gamma)^2 S_{aa} + (\Gamma^2 + k_2^2) S_{hh} + 2H\Gamma S_{fa} \quad \textbf{(4-46)}$$

$$+ (\Gamma + ik_2) (S_{fh} + H\Gamma S_{ah}) + (\Gamma - ik_2) (S_{hf} + H\Gamma S_{ha})]$$

In the special case $C_{aa} = \zeta^2 C_{ff}$, (4-29) and (4-30) are used to obtain the spectral densities of the velocity components in terms of S_{ff}:

$$S_{v1.v1} = \frac{K_m^2}{\theta^2} \frac{k_1^2 k_2^2}{(k_1^2 + k_2^2) + \Gamma^2 k_2^2} (1 + 2\rho\zeta H\Gamma + +(\zeta H\Gamma)^2) S_{ff}$$

$$\textbf{(4-47)}$$

$$S_{v2.v2} = \frac{K_m^2}{\theta^2} \left[1 - \frac{k_2^2(\Gamma^2 + k_2^2) + k_1^2 k_2^2}{(k_1^2 + k_2^2) + \Gamma^2 k_2^2}\right] (1 + 2\rho\zeta H\Gamma + +(\zeta H\Gamma)^2) S_{ff}$$

Other cross-spectral density functions involving the velocity are computed equivalently.

4.4 Obtaining 2-D (Cross-)Covariance Functions from (Cross-) Spectral Density Functions by Inverse Fast Fourier Transforms

The (cross-) covariance function $C_{pq}(\xi) = \langle X_p(\mathbf{x})\, X_q(\mathbf{x}+\xi)\rangle$ and the (cross-) spectral density function $S_{pq}(\mathbf{k})$ as used in this and previous chapters are defined by the Fourier transform pair (3-4) and (3-5) in chapter 3:

$$C_{pq}(\xi) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\xi} S_{pq}(\mathbf{k})\, d\mathbf{k} \qquad (3\text{-}4)$$

$$S_{pq}(\mathbf{k}) = \frac{1}{2\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\xi} C_{pq}(\mathbf{k})\, d\xi \qquad (3\text{-}5)$$

The inverse Fourier transforms (3-4) of the (cross-) spectral density functions derived in the previous sections are implemented numerically since a rigorous analytical evaluation of the

double Fourier integrals is very difficult if not impossible. In the past, spectral density functions derived for saturated flow and for unsaturated flow with constant α or normally distributed α have either been evaluated for ξ=0 only (Yeh et al., 1985a,b), by numerical integration (Yeh et al., 1985a,b; Russo, 1993a), or analytically for a specific class of S_{ff} (Bakr et al., 1978; Mizell, 1981). Russo (1993a) used the spectral densities of the head h' and its gradient j_n' and the cross-spectral densities involving f', a', h', and j_n' given by Yeh et al. (1985b). The respective (cross-)covariances are evaluated numerically, and the covariance functions of y', v_1', and v_2' are derived as functions (superpositions) of these numerically evaluated covariance and cross-covariances. The superposition of several numerically evaluated covariance and cross-covariance functions to obtain the unsaturated hydraulic conductivity and velocity covariances is very error prone, particularly for $C_{v2.v2}$, the covariance of the velocity component parallel to mean flow. If the numerical evaluation of the inverse Fourier transforms of the expressions in Yeh et al. (1985b) is not implemented with great accuracy, the additive errors resulting in the numerically obtained (cross-) covariances from which $C_{v2.v2}$ is computed may become considerable. In contrast, the spectral density $S_{v2.v2}$ derived here (4-46) is exact in the first order sense, and only one Fourier integral needs to be evaluated.

Unlike in the above mentioned studies, advantage is taken of a numerical technique called (inverse) "fast Fourier transform" (FFT), which has already been encountered in the previous chapter on random field generators. FFT algorithms were introduced five decades ago (Press et al., 1992). The development of their fundamental theoretical framework and various techniques for their implementation have since evolved into a field of science itself (Brigham, 1988). FFT algorithms are readily available for many computer platforms and programming languages (also see chapter 3.5). The FFT algorithm is SCFT2 provided by the Engineering and Scientific Solutions Library (ESSL) (IBM, 1993) that is part of the Fortran compiler for the IBM RS/6000 workstations.

As with all FFT algorithms, the SCFT2 algorithm is defined in terms of the spatial frequency u instead of the spectral wave-number k, where

$$k = 2\pi u \tag{4-48}$$

Introducing a new variable $\hat{S}_{pq}(\mathbf{u}) = (2\pi)^2 S_{pq}(2\pi\mathbf{u})$, substituting k with u, and noting that in two dimensions $d\mathbf{k} = (2\pi)^2 d\mathbf{u}$, the Fourier transform pair (3-4) and (3-5) becomes (compare to (3-8) and (3-9):

$$\hat{S}_{pq}(\mathbf{u}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i2\pi\mathbf{u}\cdot\xi}\, C_{pq}(\xi)\, d\xi \tag{4-49}$$

$$C_{pq}(\xi) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i2\pi\mathbf{u}\cdot\xi}\, \hat{S}_{pq}(\mathbf{u})\, d\mathbf{u} \tag{4-50}$$

In the numerical Fourier transform the continuous function under the integral is evaluated at a finite number of discrete arguments i.e., the integral is discretized into a sum, and truncated at sufficiently large positive and negative limits of the summation variable. The discretization and the truncation involve numerical errors, as will be seen later. The covariance function is discretized into a regular two-dimensional grid with an equal number of gridpoints in each direction:

$$\xi_n = n\Delta\xi \qquad n = -M, M-1 \tag{4-51}$$

Similarly, the spectral density function is discretized on a regular two-dimensional grid with an equal number of grid-points in each direction:

$$u_m = m\Delta u \qquad m = -M, M-1 \tag{4-52}$$

The spacing of the frequencies $\Delta\mathbf{u}$ is a function of the total length of the spatial grid $2M\Delta\mathbf{x}$, since the lowest possible frequency (the frequency with the longest possible wavelength) in the discretized domain has a length equal to the side-length of the spatial domain (see chapter 3.2):

$$\Delta u = \frac{1}{2M\Delta\xi} \tag{4-53}$$

Similarly the highest possible frequency or Nyquist frequency is the reciprocal of twice the spatial discretization:

$$u_M = \frac{1}{2\Delta\xi} \tag{4-54}$$

To obtain the covariance function, a spatial discretization $\Delta\xi$ must be defined *a priori*. The gridpoints are then specified by

$$u_m = \frac{m}{2M\Delta\xi} \tag{4-55}$$

and since the spectral density functions in section (3.3) are defined in terms of **k**:

$$k_m = \frac{2\pi m}{2M\Delta\xi} \tag{4-56}$$

Most numerical FFTs pack the arrays for C_{pq} and S_{pq} not from -M to M-1, but from 0 to 2M-1 such that the values from -M to -1 are packed into the area M to 2M-1. In other words, for the purpose of the FFT $\hat{S}_{pq}$ is packed as follows:

$$\begin{aligned}
&\hat{S}_{pq}(2M-m_1,2M-m_2) = \hat{S}_{pq}(-m_1,-m_2) && 1 < m_1,m_2 < M \\
&\hat{S}_{pq}(m_1,2M-m_2) = \hat{S}_{pq}(m_1,-m_2) && 1 < m_1,m_2 < M \\
&\hat{S}_{pq}(2M-m_1,m_2) = \hat{S}_{pq}(-m_1,m_2) && 1 < m_1,m_2 < M
\end{aligned} \tag{4-57}$$

and equivalently C_{pq}:

$$\begin{aligned}
&C_{pq}(2M-n_1,2M-n_2) = C_{pq}(-n_1,-n_2) && 1 < n_1,n_2 < M \\
&C_{pq}(n_1,2M-n_2) = C_{pq}(n_1,-n_2) && 1 < n_1,n_2 < M \\
&C_{pq}(2M-n_1,n_2) = C_{pq}(-n_1,n_2) && 1 < n_1,n_2 < M
\end{aligned} \tag{4-58}$$

The reasons for the packing order are explained, for example, in Brigham (1988).

Now the approximate inverse Fourier transform of S(**k**) can be obtained by replacing

the integrals in (4-49) by a double summation, expanding $\hat{S}_{pq}(\mathbf{u})$ in terms of $S_{pq}(\mathbf{k})$ and replacing d$\mathbf{u}$ by $\Delta\mathbf{u}$:

$$C_{pq}(n_1\Delta x_1, n_2\Delta x_2) =$$

$$\sum_{m_1=0}^{2M-1}\sum_{m_2=0}^{2M-1} e^{\frac{i2\pi}{2M}m_1n_1}\, e^{\frac{i2\pi}{2M}m_2n_2}\, S_{pq}\left(\frac{2\pi}{2M\Delta x_1}m_1\ ,\ \frac{2\pi}{2M\Delta x_2}m_2\right)\ \frac{2\pi}{2M\Delta x_1}\cdot\frac{2\pi}{2M\Delta x_2} \qquad \textbf{(4-59)}$$

which is the definition of the Fourier transform SCFT2 in ESSL:

$$y(n_1,n_2) =$$

$$\text{scale}\sum_{m_1=0}^{l1-1}\sum_{m_2=0}^{l2-1} x(m_1,m_2)\, e^{\text{isign}\frac{-i2\pi}{l1}m_1n_1}\, e^{\text{isign}\frac{-i2\pi}{l2}m_2n_2} \qquad \textbf{(4-60)}$$

where

$$y(n_1,n_2) = C_{pq}(n_1,n_2)$$

$$x(m_1,m_2) = S_{pq}(2\pi m_1/(2M\Delta x_1), 2\pi m_2/(2M\Delta x_2))$$

$$\text{scale} = (2\pi)^2/(4M^2\Delta x_1\Delta x_2) \qquad l1 = l2 = 2M \qquad \text{isign} = -1$$

From (4-51) and (4-52) it is seen that the discretization in the spatial domain determines the truncation in the frequency domain, while the truncation in the spatial domain determines the discretization in the frequency domain. Truncation and discretization error are therefore inseparable since both need to be avoided in both domains if the FFT is to be an accurate estimate of the Fourier integral (4-49) (see e.g. Robin et al., 1993). A discretization in the spatial domain such that $\lambda_f = 10\xi$ and $M=100\ \lambda_f$ gives a sufficiently accurate estimate of (4-49). Discretizing ξ such that $\lambda_f = 20\xi$ and $M=100\ \lambda_f$ or $\lambda_f = 10\xi$ and $M=200\ \lambda_f$ does not significantly change the results. Pseudo-analytical solutions of the covariance and cross-covariance functions obtained after a numerical FFT of the analytical spectral density functions given in this chapter are shown in subsequent chapters 6 and 8.