Sensitivity of output covariance to non-second order properties in the case of unsaturated zone models

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Abstract

The classical way of doing Monte Carlo analysis is : starting from the covariance of the input, generate a great number of possible inputs, present them to the model and deduce from all generated outputs the covariance of the output. This procedure is widely used in unsaturated zone hydrology research.

Theoretically it is clear that if the model is non-linear (and unsaturated zone models are non-linear) the covariance of the output depends also on non-covariance properties of the input.

In this paper an easy method of investigating the sensitivity of the output to the non-covariance properties of the input will be presented. The metod is based on Fourier analysis and changing the phases of transforms.

Contents

Chapter 1

Introduction

It has been recognized in the last few decades that a purely deterministic approach to describe soil water behavior may not be adequate on a scale larger than is generally used for a laboratory or small field experiments. Especially, Monte Carlo technique has been frequently applied to simulate flow and transport in microscopically heterogeneous soil structures . There is a long tradition of using this method to study a chemical transport in aquifers, however, only recently has it been applied to examine physical processes in the unsaturated zone (see,e.g., Cislerova [2]).

In the most of the reported studies the Monte Carlo analysis has been used to express soil water pressure head, water content, flux or the other output dynamical variables from the unsaturated zone deterministic - nonlinear models as a stochastic function of the second order properties of the soil medium (see, e.g., Roth [9] , Russo[10], Hopmans et al. [4]). It is widely accepted that the analysis gives direct (statistical, based on second order properties) insight in how the output variables are controlled by spatial variability of soil parameters provided that statistical (second order) properties of the parameters are given and reflect the real field variability. On the other hand, it is theoretically clear that if the model is nonlinear the covariance of the output depends also on non-covariance properties of the input. An examination of sensitivity of the output covariance structure to non-second order properties of the input based on spectral Fourier analysis clearly illustrates limitations of the classical Monte Carlo approach.

Chapter 2

Random fields

It is very intuitive to associate the term "random field " with a giant laboratory where investigator can do numerous experiments. Observing the outcome of all the experiments in the laboratory is equivalent to observing the realization of the random field. The location of each experimental setup in the laboratory is identified , in the terminology of random fields by, a set of "coordinates ". In a simple experiment the investigator may observe the value of the random field at one specific location, or simultaneously two, three or more values at different locations. The outcome of the experiment is called realization of the random field.

After having intuition built up, in this chapter the more precise definition and basic properties of random fields that are neccesary to understand the analysis done in this project will be given. To get familiar with spectral techniques used, some important aspects of classical random field analysis in frequency domain will be reflected as well. Mathematics presented in this chapter mostly refers to two standard textbooks on generalized stochastic processes theory, namely Priestley[8] and Vanmarcke[13] Without loss of generality we limited our considerations to 2-D index space.

2.0.1 Definitions

Let us suppose that the stochastic quantity which we are studying varies over space, so that we may denote it by $\mathbf{Z}(\mathbf{x})$. Then at each individual space point $\mathbf{x}$, $\mathbf{Z}(\mathbf{x})$ is a random variable.

Definition 1 *A random (or stochastic) field , $\{\mathbf{Z}(\mathbf{x})\}$, is a family of random variables indexed by the symbol $\mathbf{x}$, where $\mathbf{x}$ belongs to some given index*

set $\mathbf{X}$.

Definition 2 *If it takes a continuous range of real values (finite or infinite), so that* $\mathbf{X} \subseteq \mathbf{R}^2$, $\{\mathbf{Z}(\mathbf{x}) : \mathbf{x} \in \mathbf{X}\}$ *is said to be a continuous field. If elements of* $\mathbf{x}$ *(coordinates of a point in* $\mathbf{R}^2$*) take a discrete set of values, then* $\{\mathbf{Z}(\mathbf{x})\}$ *is said to be a discrete field.*

2.0.2 Realizations and ensembles

The fact that for each $\mathbf{x}$, $\mathbf{Z}(\mathbf{x})$ is a random variable means that each time we perform an experiment we will, in general, observe a different value of $\mathbf{Z}(\mathbf{x})$. Thus an observed record of a random field is merely one record out of the whole collection of all possible records which we might have observed. The collection of all possible records is called the *ensemble* , and each particular record is called a *realization* of the field. Differences between the realizations provide a measure of spatial uncertainty

We may think of the sample space $\mathbf{\Omega}$, as consisting of a set of elements $\{\omega\}$ each of which corresponds to a particular realization, and we may then denote the various realizations by $\{\mathbf{Z}(\mathbf{x},\omega_1)\}, \{\mathbf{Z}(\mathbf{x},\omega_2)\}, ...,$ and a typical realization by $\{\mathbf{Z}(\mathbf{x},\omega)\}$ or just by $\mathbf{z}(\mathbf{x})$. With this notation the random field itself would be written as $\{\mathbf{Z}(\mathbf{x},\cdot)\}$, but it is just more convenient to suppress the variable (ω) and denote a random field simply by $\{\mathbf{Z}(\mathbf{x})\}$.

2.0.3 General specification of a random field

For each $\mathbf{x}$, $\mathbf{Z}(\mathbf{x})$ is a random variable and thus has a range of possible values, some of which may be more likely to occur than the others. Accordingly, for each $\mathbf{x}$, $\mathbf{Z}(\mathbf{x})$ will have a probability distribution function $f_{\mathbf{Z}(\mathbf{x})}(\cdot)$ defined.

The above approach enables us to discuss the probability distribution of $\mathbf{Z}(\mathbf{x})$ for *each individual value* $\mathbf{x}$. However, since we are dealing with a collection of random variables (corresponding to the values of the field at all points in space) we may wish to study the joint variation of the values of the field at all space points. To do this we need to know the joint probability distribution of all the random variables $\{\mathbf{Z}(\mathbf{x}_0), \mathbf{Z}(\mathbf{x}_1), ..., \mathbf{Z}(\mathbf{x}_{m-1})\}$. In the case of continuous random field we have to deal with an infinite dimensional joint probability distribution. But in practical situations only discrete random fields are considered so the joint distribution is finite dimensional..

Theorem 3 *For any positive integer m let* $\mathbf{x}_0, \mathbf{x}_1, ..., \mathbf{x}_{m-1}$ *be any admissible set of elements of* $\mathbf{x}$. *Then under general conditions the probabilistic structure of the random field* $\{\mathbf{Z}(\mathbf{x})\}$ *is completely specified if we are given the joint probability distribution of* $(\mathbf{Z}(\mathbf{x}_0), \mathbf{Z}(\mathbf{x}_1), ..., \mathbf{Z}(\mathbf{x}_{m-1}))$ *for all values of m and for all choices of* $\mathbf{x}_0, \mathbf{x}_1, ..., \mathbf{x}_{m-1}$.

2.0.4 Moments

Let $\mathbf{Z}(\mathbf{x})$ be a random variable with a 1 - dimensional probability density function $f_{\mathbf{Z}(\mathbf{x})}(\zeta)$. The mean and variance of $f_{\mathbf{Z}(\mathbf{x})}(\zeta)$ are defined as :

$$\mathbf{E}\left[\mathbf{Z}(\mathbf{x})\right] = \int_{-\infty}^{\infty} \zeta f_{\mathbf{Z}(\mathbf{x})}(\zeta) d\zeta = \mu(\mathbf{x}) \tag{2.1}$$

$$\mathbf{Var}\left[\mathbf{Z}(\mathbf{x})\right] = \mathbf{E}\left[\{\mathbf{Z}(\mathbf{x}) - \mu(\mathbf{x})\}^2\right] = \int_{-\infty}^{\infty} (\zeta - \mu(\mathbf{x}))^2 \ f_{\mathbf{Z}(\mathbf{x})}(\zeta) d\zeta = \sigma^2(\mathbf{x}) \tag{2.2}$$

The above specified quantities are extremely useful in providing a rough summary of the form of probability distribution. However, it should be clear that the two numbers could never fully describe the $f(\mathbf{Z}(\mathbf{x}))$ function. Indeed, there are many distributions with exactly the same $\mu(\mathbf{x})$ and $\sigma^2(\mathbf{x})$ but with shapes differing in other respects. To characterize them we need to define somewhat more general sequence of constants. The constants are called nth order moments. They can be divided in two groups: rth moments about the origin given by:

$$\mathbf{E}\left[\mathbf{Z}(\mathbf{x})^n\right] = \int_{-\infty}^{\infty} \zeta^n f_{\mathbf{Z}(\mathbf{x})}(\zeta) d\zeta = \mu_n'(\mathbf{x}) \tag{2.3}$$

and rth order moments centralized about the mean :

$$\mathbf{E}\left[\widehat{\mathbf{Z}(\mathbf{x})}^n\right] = \int_{-\infty}^{\infty} \widehat{\zeta}^n f_{\mathbf{Z}(\mathbf{x})}(\zeta) d\zeta = \mu_n(\mathbf{x}) \tag{2.4}$$

where:

$$\widehat{\mathbf{Z}(\mathbf{x})} = \mathbf{Z}(\mathbf{x}) - \mu(\mathbf{x})$$

Straightforwardly, on can see:

$$\mu_1^{'}(\mathbf{x}) = \mu(\mathbf{x}) \tag{2.5}$$

$$\mu_2(\mathbf{x}) = \sigma^2(\mathbf{x}) \tag{2.6}$$

In a similar way joint moments that characterize the joint probability distribution $f_{\mathbf{Z(x_0)},\mathbf{Z(x_1)},...,\mathbf{Z(x_{m-1})}}(\zeta_0\zeta_1...\zeta_{m-1})$of $\{\mathbf{Z(x)}\}$are defined as :

$$E[\mathbf{Z}(\mathbf{x}_0)^{n_0}\mathbf{Z}(\mathbf{x}_1)^{n_1}...\mathbf{Z}(\mathbf{x}_{m-1})^{n_{m-1}}] =$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}...\int_{-\infty}^{\infty}\zeta_0{}^{n_0}\zeta_1{}^{n_1}...\zeta_{m-1}{}^{n_{m-1}}\ f_{\mathbf{Z(x_0)},\mathbf{Z(x_1)},...,\mathbf{Z(x_{m-1})}}(\zeta_0{}^{n_0},\zeta_1{}^{n_1},...,\zeta_{m-1}{}^{n_{m-1}})d\zeta_0\zeta_1...\zeta_{m-1} \tag{2.7}$$

and

$$E[\widehat{\mathbf{Z}(\mathbf{x}_0)}^{n_0}\widehat{\mathbf{Z}(\mathbf{x}_1)}^{n_1}...\widehat{\mathbf{Z}(\mathbf{x}_{m-1})}^{n_{m-1}}] =$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}...\int_{-\infty}^{\infty}\widehat{\zeta}_0{}^{n_0}\widehat{\zeta}_1{}^{n_1}...\widehat{\zeta}_{m-1}{}^{n_{m-1}}\ f_{\mathbf{Z(x_0)},\mathbf{Z(x_1)},...,\mathbf{Z(x_{m-1})}}(\zeta_0{}^{n_0},\zeta_1{}^{n_1},...,\zeta_{m-1}{}^{n_{m-1}})d\zeta_0\zeta_1...\zeta_{m-1} \tag{2.8}$$

for positive integers $n_0, n_{1,...,}n_{m-1}$satisfying $n_0+n_1+...+n_{m-1} \leq n$. Setting $n_0, n_1 = 1$ and the remaining n's to 0 we are able to define *covariance function* $B(\mathbf{x},\mathbf{x}')$ that characterizes the variation of a random field at two locations: $\mathbf{x}$ and $\mathbf{x}'$.

$$B(\mathbf{x},\mathbf{x}') \equiv \mathbf{Cov}\left[\mathbf{Z}(\mathbf{x}),\mathbf{Z}(\mathbf{x}')\right] = \mathbf{E}\left[\mathbf{Z}(\mathbf{x})\mathbf{Z}(\mathbf{x}')\right] - \boldsymbol{\mu}(\mathbf{x})\boldsymbol{\mu}(\mathbf{x}') \tag{2.9}$$

or the *correlation function*

$$\rho(\mathbf{x},\mathbf{x}') \equiv \rho_{\mathbf{Z}}(\mathbf{x},\mathbf{x}') = \frac{B(\mathbf{x},\mathbf{x}')}{\sigma(\mathbf{x})\sigma(\mathbf{x}')} \tag{2.10}$$

where $\boldsymbol{\mu}(\mathbf{x})$ and $\boldsymbol{\mu}(\mathbf{x}')$ are the means and $\sigma(\mathbf{x})$ and $\sigma(\mathbf{x}')$ are the standard deviations of $\mathbf{Z}(\mathbf{x})$ and $\mathbf{Z}(\mathbf{x}')$ respectively.

2.0.5 Gaussian fields

Of special interest are the random fields whose multivariate distributions are normal. These fields are called *Gaussian random fields.*

Their probabilistic structure is given by the multivariate normal probability density function :

$$f_{\mathbf{Z}(\mathbf{x}_0),\mathbf{Z}(\mathbf{x}_1),\ldots,\mathbf{Z}(\mathbf{x}_{m-1})}(\zeta_0\zeta_1\cdots\zeta_{m-1}) = (2\pi)^{-\left(\frac{m}{2}\right)} \left|\underline{\underline{\mathbf{B}}}\right|^{-\left(\frac{1}{2}\right)} \exp\left\{-\frac{1}{2}\left(\underline{\zeta}-\underline{\mu(\zeta)}\right)^T \underline{\underline{\mathbf{B}}}^{-1}\left(\underline{\zeta}-\underline{\mu(\zeta)}\right)\right\} \tag{2.11}$$

where:

$$\underline{\underline{\mathbf{B}}} = \mathbf{Cov}\left[\mathbf{Z}(\mathbf{x}_k), \mathbf{Z}(\mathbf{x}_l)\right]; \quad k,l = 0,\ldots,m-1 \tag{2.12}$$

$$\underline{\zeta} = \begin{bmatrix} \zeta_0 \\ \zeta_1 \\ \cdot \\ \cdot \\ \zeta_{m-1} \end{bmatrix}, \underline{\mu(\zeta)} = \begin{bmatrix} \mu(\zeta_0) \\ \mu(\zeta_1) \\ \cdot \\ \cdot \\ \mu(\zeta_{m-1}) \end{bmatrix} \tag{2.13}$$

2.1 Properties and assumptions

A continuous random field usually contains an infinite and uncountable number of points. In discrete case the number of points is finite but always very large. However, there is never enough data to validate fully assumed multivariate probability distributions. Several key properties of random fields - homogeneity, isotropy and ergodicity - permit the analyst to make more efficient use of what little data are available to estimate probability distributions and their statistics.

2.1.1 Homogeneity - stationarity in space

Strict stationarity

The physical fields that are characterized by the feature that their statistical properties do not change over space are termed "stationary " or "homogeneous ".

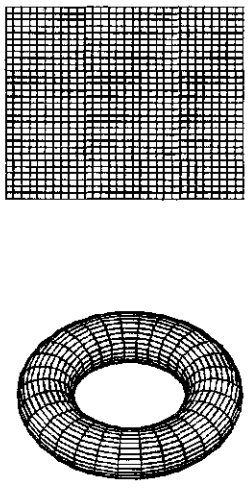

Figure 2.1: A lattice on which a discrete random field is generated may be represented as a torus surface. That makes shifts possible

Definition 4 *The field* $\{\mathbf{Z}(\mathbf{x})\}$ *is said to be strict stationary or complete stationary if, for any admissible* $\mathbf{x}_0, \mathbf{x}_1, ..., \mathbf{x}_{m-1}$ *and any* Δ *, the joint probability distribution of* $(\mathbf{Z}(\mathbf{x}_0), \mathbf{Z}(\mathbf{x}_1), ..., \mathbf{Z}(\mathbf{x}_{m-1}))$ *is identical with the joint probability distribution of* $(\mathbf{Z}(\mathbf{x}_0 + \Delta), \mathbf{Z}(\mathbf{x}_1 + \Delta), ..., \mathbf{Z}(\mathbf{x}_{m-1} + \Delta))$ *, i.e. if*

$$f_{\mathbf{Z}(\mathbf{x}_0),\mathbf{Z}(\mathbf{x}_1),...,\mathbf{Z}(\mathbf{x}_{m-1})}(\zeta_0\zeta_1\cdots\zeta_{m-1}) \equiv f_{\mathbf{Z}(\mathbf{x}_0+\Delta),\mathbf{Z}(\mathbf{x}_1+\Delta),...,\mathbf{Z}(\mathbf{x}_{m-1}+\Delta)}(\zeta_0\zeta_1\cdots\zeta_{m-1}) \tag{2.14}$$

where $f_{\mathbf{Z}(\mathbf{x}_0),\mathbf{Z}(\mathbf{x}_1),...,\mathbf{Z}(\mathbf{x}_{m-1})}(\cdot)$ *denotes the probability density function of the set of random variables which appear as suffixes.*

Remark 1 *To make the shifts* Δ *possible in a finite space one may think about the field* $\{\mathbf{Z}(\mathbf{x})\}$ *as a torus (see Fig.2.1). Then, for any* $\mathbf{x} = (x_1, x_2)$ *and* $\Delta = (\Delta_1, \Delta_2)$ *we have:*

$$\mathbf{x}+\Delta = (x_1, x_2) + (\Delta_1, \Delta_2) = ((x_1 + \Delta_1) \bmod M), (x_2 + \Delta_2) \bmod N)$$
$$\text{where } x_1 = 0; ..., M-1 \text{ and } x_2 = 0; ..., N-1$$

The property described by Equation 2.14 may be summarized by saying that *the probabilistic structure of a strict stationary field is invariant under a shift of the coordinate system origin.*

Weak stationarity

In practice, random fields that are assumed to possess stationarity property do so in a limited or weak sense, not in the strict sense. The fields are then called *stationary up to order n* . Under this weaker condition ,e.g., the probability distribution of $\mathbf{Z}(\mathbf{x}_0)$ does not have to be identical to the probability distribution of $\mathbf{Z}(\mathbf{x}_0 + \Delta)$, but the main features of these two distributions should be the same, i.e.e their moments up to a certain order, should be the same.

Definition 5 *The field* $\mathbf{Z}(\mathbf{x})$ *is said to be stationary up to order m if, for any admissible* $\mathbf{x}_0, \mathbf{x}_1, ..., \mathbf{x}_{m-1}$ *and any* Δ *, all the joint moments up to order n of* $(\mathbf{Z}(\mathbf{x}_0), \mathbf{Z}(\mathbf{x}_1), ..., \mathbf{Z}(\mathbf{x}_{m-1}))$ *exist and equal the corresponding joint moments up to order n of* $(\mathbf{Z}(\mathbf{x}_0 + \Delta), \mathbf{Z}(\mathbf{x}_1 + \Delta), ..., \mathbf{Z}(\mathbf{x}_{m-1} + \Delta))$.

Thus,

$$E[\mathbf{Z}(\mathbf{x}_0)^{n_0}\mathbf{Z}(\mathbf{x}_1)^{n_1}...\mathbf{Z}(\mathbf{x}_{m-1})^{n_{m-1}}] = E[\mathbf{Z}(\mathbf{x}_0+\Delta)^{n_0}\mathbf{Z}(\mathbf{x}_1+\Delta)^{n_1}...\mathbf{Z}(\mathbf{x}_{m-1}+\Delta)^{n_{m-1}}] \tag{2.15}$$

for any Δ, and all positive integers $n_0, n_{1,...,}n_{m-1}$satisfying $n_0 + n_1 + ... + n_{m-1} \leq n$. In particular , setting $n_1 = n_2 = ... = n_{m-1} = 0$,we have that for any t and all $n_0 \leq n$,

$$\begin{aligned} \mathbf{E}\left[\mathbf{Z}(\mathbf{x})^{n_0}\right] &= \mathbf{E}\left[\mathbf{Z}(\mathbf{0})^{n_0}\right] \qquad (\text{taking } \Delta = -\mathbf{x}\ ) \\ &= \text{a constant, independent on } \mathbf{x} \end{aligned} \tag{2.16}$$

Also for any $\mathbf{x}, \mathbf{x}'$ and all n_0, n_1 satisfying $n_0 + n_1 \leq n$,

$$\begin{aligned} \mathbf{E}\left[\mathbf{Z}(\mathbf{x})^{n_0}\mathbf{Z}(\mathbf{x}')^{n_1}\right] &= \mathbf{E}\left[\mathbf{Z}(\mathbf{0})^{n_0}\mathbf{Z}(\mathbf{x}'-\mathbf{x})^{n_1}\right] \\ &= \text{function of } (\mathbf{x}'-\mathbf{x}) \text{ only} \end{aligned} \tag{2.17}$$

Now let us define stationarity up to order 2 (n=2) as it has been assumed in this study.

Definition 6 *The field* $\mathbf{Z}(\mathbf{x})$ *is stationary up to order 2 if*

- $\mathbf{E}\left[\mathbf{Z}(\mathbf{x})\right] = \mu(\mathbf{x}) = \mu$, *a constant independent on* $\mathbf{x}$

- $\mathbf{E}\left[\mathbf{Z}^2(\mathbf{x})\right] = \xi^2$, *a constant independent on* $\mathbf{x}$ *(using Equation2.16 with* $n_0 = 2$*)*

  Hence, $\mathbf{Var}\left[\mathbf{Z}(\mathbf{x})\right] = \xi^2 - \mu^2 = \sigma^2$, *is also constant independent on* $\mathbf{x}$

  Further, for any $\mathbf{x}, \mathbf{x}'$,

- $\mathbf{E}\left[\mathbf{Z}(\mathbf{x})\mathbf{Z}(\mathbf{x}')\right]$ = *function of* $(\mathbf{x}' - \mathbf{x})$ *only (using Equation 2.17 with* $n_0, n_1 = 1$*).*

  Hence, $\mathbf{Cov}\left[\mathbf{Z}(\mathbf{x}), \mathbf{Z}(\mathbf{x}')\right] = \mathbf{E}\left[\mathbf{Z}(\mathbf{x})\mathbf{Z}(\mathbf{x}')\right] - \mu^2 = \mathbf{Cov}(\mathbf{x}' - \mathbf{x})$ *function of* $(\mathbf{x}' - \mathbf{x})$ *only.*

2.1.2 Isotropy

Definition 7 *The field* $\mathbf{Z}(\mathbf{x})$ *is isotropic if the joint probability density functions remain the same even when the constellation of points* $\mathbf{x}_0, \mathbf{x}_1, ..., \mathbf{x}_{m-1}$ *is rotated .*

The above definition, however, applies only to continuous fields : simply if lattice -defined discrete field is rotated we will obtain a different lattice then the previous one. In the case of discrete fields we might only try to mimic the isotropy property by introducing covariance function that depends only on distance (see Section2.2.1) and by dense discretization what was done in this project .

2.1.3 Ergodicity hypotesis

The conceptual difficulty in most practical applications of random fields theory is that one deals only with a single realization of the field. The statistical information over the ensemble has to be based upon that single realization, since no other information is available. To make it possible one has to assume so called ergodicity property.

Definition 8 *A random field* $\mathbf{Z}(\mathbf{x})$ *is ergodic if all information about joint probability distributions (and their statistics) can be obtained from a single realization of the random field. Explicitly :*

$$E\left[\mathbf{Z}(\mathbf{x})\right] = \lim_{S \to \infty} \frac{1}{|S|} \int_S \mathbf{Z}(\mathbf{x}) d\mathbf{x} \tag{2.18}$$

Ergodicity is a generalization of the well known low of large numbers that states that for independent, identically distributed drawings of a stochastic variable the sample mean converges to the population mean.

The two means are simply replacable if ergodicity is assumed.

Stationarity often guarantees ergodicity. We can test for homogeneity of the field by dividing the field into parts and see weather the statistical information for the parts is the same or not. If they are the same, the field is homogeneous and ergodicity may be assumed

2.2 Second order analysis

2.2.1 Covariance function of a homogeneous random field

General information

If the random field is homogeneous, its covariance function will depend only on the relative position of the points $\mathbf{x}$ and $\mathbf{x}'$, and we may write:

$$B(\mathbf{x}, \mathbf{x}') = B(\mathbf{x} - \mathbf{x}') = B(\boldsymbol{\chi}) = B(\chi_0, \chi_1) \tag{2.19}$$

where $\boldsymbol{\chi} = \mathbf{x} - \mathbf{x}'$ is the lag vector whose components are $\chi_k = x_k - x'_k$ for $k = 0, 1$.

2 - dimensional covariance function of a homogeneous random field can be represented by two functions , both defined for positive lags only:

$$B(\chi_0, \chi_1) = B(-\chi_0, -\chi_1), \qquad \chi_0, \chi_1 \geq 0 \tag{2.20}$$

and

$$\overline{B}(\chi_0, \chi_1) = B(-\chi_0, \chi_1) = B(\chi_0, -\chi_1), \qquad \chi_0, \chi_1 \geq 0 \tag{2.21}$$

Likewise for n-dimensional field there are 2^{n-1} such functions defined for $\boldsymbol{\chi} \geq 0$ only. It is evident that the same can be said for the normalized covariance function $\rho(\boldsymbol{\chi})$.

Quadrant symmetry

Of considerable practical importance is the class of homogeneous random fields whose covariance function is *even* with respect to each component of the lag vector :

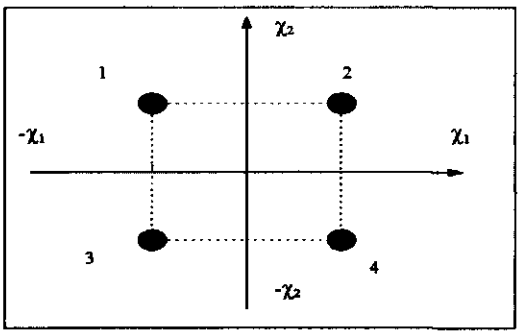

Figure 2.2: Four point pattern illustrates the concept of quadrant symmetry.

$$B(\chi_0, \chi_1) = B(-\chi_0, -\chi_1) \tag{2.22}$$

Random fields whose covariance function obeys Equation 2.22 will be called *quadrant symmetric (q.s.)* . Quadrant symmetry implies homogeneity in the weak sense. For q.s. fields the covariance function *defined for positive lags only* fully represents the covariance structure of $\mathbf{Z}(\mathbf{x})$, since information from one quadrant of the lag space suffices to describe the multidimensional covariance structure .

In reference to figure 2.2 , it means that the covariance of values associated with points 1,2,3,4 must be the same at all the points.

Isotropic covariance structure

If the covariance function depends only on the distance χ between points x and x'

$$\chi = |\boldsymbol{\chi}| = |\mathbf{x} - \mathbf{x}'| = \left[\chi_0^2 + \chi_1^2\right]^{\frac{1}{2}} \tag{2.23}$$

$B(\boldsymbol{\chi})$ will have spherical symmetry which implies quadrant symmetry. Also

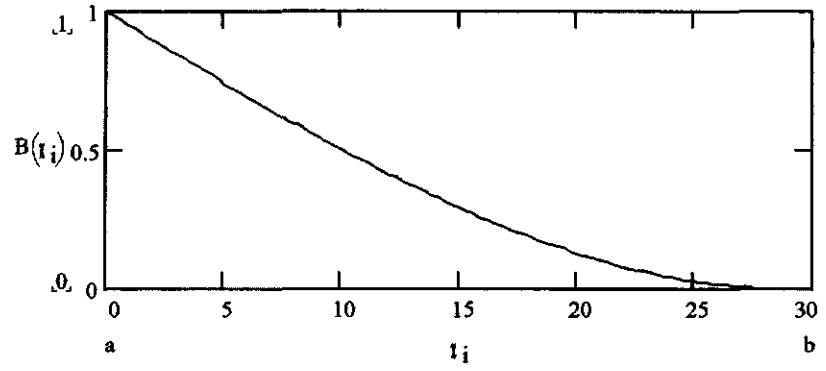

Figure 2.3: An example of radial covariance structure

$$B(\chi) \equiv B(\chi_0, \chi_1) = B(\chi, 0) = B(\chi) \equiv B^R(\chi) \tag{2.24}$$

where $B(\chi) \equiv B^R(\chi)$ is the covariance function of random process *on the line* (in any direction); $B^R(\chi)$ may be called *radial covariance function.* Therefore, if a random field is homogeneous and isotropic, the whole information neccesery to describe multidimensional covariance structure will be contained on one line of the lag space. The isotropic covariance structure was the only one we used during this research. There was simply not enough data to take anisotropy into account. To exemplify the isotropy concept, let us consider 2 - dimensional stationary and isotropic random field with radial spherical covariance function given by:

$$B^R(\chi) = \begin{matrix} 1 - \frac{3}{2}\left(\frac{\chi}{r}\right) + \frac{1}{2}\left(\frac{\chi}{r}\right)^3 \text{ if } \chi < r \\ 0 \text{ if } \chi \geq r \end{matrix} \tag{2.25}$$

where r is a range parameter (see fig 2.3). This 1 - dim function is enough to describe 2 - dim covariance structure (homogeneous and isotropic) presented on fig 2.4.

2.2.2 Estimation of mean and covariance based on ergodic assumption

A natural estimate of $\mu(\mathbf{x})$ for 2 -D discrete, stationary and ergodic realization of the Gaussian random field (discretized on $n \times m$ lattice where

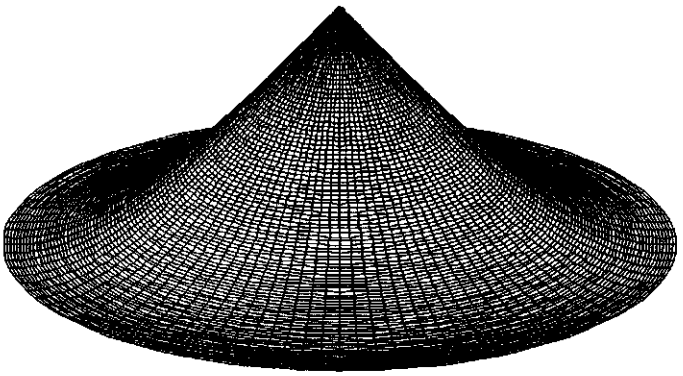

Figure 2.4: 2-D spherical covariance surface

$n = 0, ..., N-1$ and $m = 0, ..., M-1$) $\mathbf{Z}(n, m)$ is given by the sample mean:

$$\widehat{\mu} = \frac{1}{N \cdot M} \sum_{n=0}^{N-1} \sum_{m=0}^{M-1} \mathbf{Z}(n, m) \tag{2.26}$$

Similarly a natural estimate of the realization of covariance structure $B(\boldsymbol{\chi})$ is given by

$$\widehat{B}(n, m) = \frac{1}{N \cdot M} \sum_{\chi_1=0}^{N-1} \sum_{\chi_2=0}^{M-1} \mathbf{Z}(n, m) \cdot \mathbf{Z}(n + \chi_1, m + \chi_2) \tag{2.27}$$

In many practical situations one usually estimates the covariance structure from one particular realization of the considered field. Afterwards a theoretical parametric model is fitted (e.g. see Equation 2.25) that , as we believe, properly describes underlying covariance structure.

2.2.3 Short summary

The random fields that have been generated and analyzed in this study are assumed to be:

- real (not complex)

- two dimensional (2-D index space)
- discrete (as an approximation of continuous fields)
- Gaussian
- stationary up to second order (thus strictly stationary if the fields are Gaussian)
- isotropic
- ergodic

Under the assumptions the random field $\{\mathbf{Z}(\mathbf{x})\}$ is fully described by 1 - dimensional probability distribution and the radial covariance structure $B^R(\chi)$

Remark 2 *The properties mentioned above, excluding Gaussianity, hold for an arbitrary "elementwise " function* $\tilde{\mathbf{Z}}(x) = f(\mathbf{Z}(\mathbf{x}))$ *for all* $\mathbf{x}$

Chapter 3

Spectral representation of random fields

The basic formulas that characterize the second order properties of a stationary random fields in the frequency domain may be derived in several alternative ways. The more formal approach introduces negative as well as positive frequencies and assumes the random field to be complex, while the more physical approach, that will be used in this section, avoids complex numbers algebra and considers only non-negative frequencies.

3.1 Introduction : 2 -D discrete Fourier transform

Under reasonable conditions (see Vanmarcke[13] p. 84-85) , 2 -D discrete stationary, mean- centralized Gaussian random field (given on $n \times m$ lattice where $n = 0, ..., N-1$ and $m = 0, ..., M-1$ $\mathbf{Z}(n, m)$ may also be considered to be the double sum of cosine functions that extend to $N-1$ and $M-1$ respectively. The field may then be represented as a function of spatial frequencies $\tilde{\mathbf{Z}}(\omega_1, \omega_2)$, which allows us to study the field in *frequency domain.* The relationship between these two representations is given by the *Fourier transform* equations:

$$\mathcal{F}(\mathbf{Z}(n,m)) = \tilde{\mathbf{Z}}(\omega_1, \omega_2) = \frac{1}{NM} \sum_{n=0}^{N-1} \sum_{m=0}^{M-1} \mathbf{Z}(n,m)\, e^{(\frac{-2\pi i \omega_1 n}{N} - \frac{-2\pi i \omega_2 m}{M})} \quad (3.1)$$

$$\mathcal{F}^{-1}(\tilde{\mathbf{Z}}(\omega_1,\omega_2)) = \mathbf{Z}(n,m) = \sum_{\omega_1=0}^{N-1}\sum_{\omega_2=0}^{M-1} \tilde{\mathbf{Z}}(\omega_1,\omega_2)\; e^{(\frac{2\pi i\omega_1 n}{N}+\frac{2\pi i\omega_2 m}{M})} \tag{3.2}$$

$$\begin{aligned} \omega_1 &= 0,...,N-1 \\ \omega_2 &= 0,...,M-1 \end{aligned}$$

We can also write $\mathbf{Z}(n,m)$ as:

$$\mathbf{Z}(n,m) = \mu + \sum_{\omega_1=0}^{N-1}\sum_{\omega_2=0}^{M-1} \mathbf{C}(\omega_1,\omega_2)\cos(\omega_1 n + \omega_2 m + \boldsymbol{\phi}(\omega_1,\omega_2)) \tag{3.3}$$

where

$$\mathbf{C}(\omega_1,\omega_2) = \left|\tilde{\mathbf{Z}}(\omega_1,\omega_2)\right| \tag{3.4}$$

is the random amplitude, and

$$\boldsymbol{\phi}(\omega_1,\omega_2) = \arg(\tilde{\mathbf{Z}}(\omega_1,\omega_2)) \tag{3.5}$$

the random phase angle with spatial frequencies ω_1,ω_2.

3.2 Amplitudes and phases as spatial random variables

Since $\mathbf{Z}(n,m)$ is Gaussian all amplitudes and phase angles are mutually independent (see Equation 3.10) . Amplitudes are normally distributed and each phase angle is uniformly distributed over the range $(-\pi;\pi)$.

Remark 3 *For non - Gaussian fields phases and amplitudes are uncorrelated*

Each elementary random component $\mathbf{C}(\omega_1,\omega_2)\cos(\omega_1 n+\omega_2 m+\phi(\omega_1,\omega_2))$ has mean zero and variance:

$$\begin{aligned}\sigma^2(\omega_1,\omega_2) &= E\left[\left(\mathbf{C}(\omega_1,\omega_2)\cos(\omega_1 n+\omega_2 m+\boldsymbol{\phi}(\omega_1,\omega_2))\right)^2\right] \\ &= E\left[\mathbf{C}^2(\omega_1,\omega_2)\right]E\left[\cos^2(\omega_1 n+\omega_2 m+\boldsymbol{\phi}(\omega_1,\omega_2))\right] \\ &= \frac{1}{2}E\left[\mathbf{C}^2(\omega_1,\omega_2)\right] \qquad (3.6)\end{aligned}$$

because

$$E\left[\cos^2(\omega_1 n+\omega_2 m+\phi(\omega_1,\omega_2))\right]= \qquad (3.7)$$

$$=\frac{1}{2\pi}\int_{-\pi}^{\pi}\cos^2(\omega_1 n+\omega_2 m+\phi(\omega_1,\omega_2))d\phi(\omega_1,\omega_2)=\frac{1}{2}$$

Consequently, 2 - dim spectral density function , also called power spectrum of the field, is introduced as follows:

$$S(\omega_1,\omega_2)=\frac{1}{2}E\left[\mathbf{C}^2(\omega_1,\omega_2)\right] \qquad (3.8)$$

Since the variance of the sum of independent random functions equals the sum of their variances we can write:

$$\sigma^2=E\left[(\mathbf{Z}(n,m)-\mu)^2\right]=\sum_{\omega_1=0}^{N-1}\sum_{\omega_2=0}^{M-1}\frac{1}{2}E\left[\mathbf{C}^2(\omega_1,\omega_2)\right]= \qquad (3.9)$$

$$=\sum_{\omega_1=0}^{N-1}\sum_{\omega_2=0}^{M-1}S(\omega_1,\omega_2)\Delta\omega_1\Delta\omega_2$$

3.3 The Wiener - Khinchine relations

By introducing Equation 2.19 into the definition of bivariate covariance structure $B(\chi_0,\chi_1)$,accounting the fact that the random components $\mathbf{C}(\omega_1,\omega_2)\cos(\omega_1 n+\omega_2 m+\phi(\omega_1,\omega_2))$ are mutually independent and inserting Equation 3.3, one obtains:

$$B(\chi_0,\chi_1)=Cov\left[\mathbf{Z}(0,0)\,\mathbf{Z}(\chi_0,\chi_1)\right]=$$

$$= \sum_{\omega_1=0}^{N-1} \sum_{\omega_2=0}^{M-1} E\left[\left(\mathbf{C}\left(\omega_1,\omega_2\right)\cos(\phi\left(\omega_1,\omega_2\right))\right)\left(\mathbf{C}\left(\omega_1,\omega_2\right)\cos(\omega_1\chi_0+\omega_2\chi_1+\phi\left(\omega_1,\omega_2\right))\right)\right]$$

$$= \sum_{\omega_1=0}^{N-1} \sum_{\omega_2=0}^{M-1} E\left[\mathbf{C}^2\left(\omega_1,\omega_2\right)\right]\left(\frac{1}{2\pi}\int_{-\pi}^{\pi}\cos(\omega_1\chi_0+\omega_2\chi_1+\phi\left(\omega_1,\omega_2\right))\cos\phi\left(\omega_1,\omega_2\right)d\phi\left(\omega_1,\omega_2\right)\right)$$

$$= \sum_{\omega_1=0}^{N-1} \sum_{\omega_2=0}^{M-1} \frac{1}{2} E\left[\mathbf{C}^2\left(\omega_1,\omega_2\right)\right]\cos\left(\omega_1\chi_0+\omega_2\chi_1\right) \tag{3.10}$$

Of a great importance is the fact that the Equation 3.10 formally proves that the *covariance structure is independent on phases* .

By inserting Equation 3.8 one obtains the first relation of the 2 - dimensional Wiener - Khinchine relations :

$$B(\chi_0,\chi_1) = \sum_{\omega_1=0}^{N-1} \sum_{\omega_2=0}^{M-1} S(\omega_1,\omega_2)\cos\left(\omega_1\chi_0+\omega_2\chi_1\right) \tag{3.11}$$

$$S(\omega_1,\omega_2) = \frac{1}{NM} \sum_{\chi_0=0}^{N-1} \sum_{\chi_1=0}^{M-1} B(\chi_0,\chi_1)\cos\left(\omega_1\chi_0+\omega_2\chi_1\right) \tag{3.12}$$

which, in more formal representation take the form of Fourier transform pair :

$$B(\chi_0,\chi_1) = \mathcal{F}^{-1}(S(\omega_1,\omega_2)) \tag{3.13}$$

$$S(\omega_1,\omega_2) = \mathcal{F}(B(\chi_0,\chi_1))$$

3.3.1 Conclusions concerning Gaussian fields

For Gaussian fields the following properties hold:

1. the phases are independent, uniformly distributed and independent of amplitudes

2. amplitudes are Gaussian distributed and independent

As a consequence Gaussian fields are completely determined by power spectrum $S(\omega_1,\omega_2)$

Chapter 4

Methods and procedures

4.1 Materials

To illustrate new approach to deterministic unsaturated zone model sensitivity testing we generated random fields of one particular soil parameter : scaling factor for hydraulic conductivity. First part of this section gives a theoretical explanation of physical meaning of the parameter . In second part, data from an experiment conducted by Hopmans at al [3] at Hupselse Beek catchment, we used during input generation are presented.

4.1.1 Hydraulic conductivity scaling factor - some theory.

The theory of scaling is based on the similar media concept, introduced by Miller and Miller [6]. A general purpose of developing this procedure was to describe a stochastic nature of soil variables fields using one - parameter representation (a field of just one parameter). Similar media differ only in the scale of their internal microscopic geometries and have therefore equal porosities and equivalent particle and pore-size distributions. The purpose of scaling is to simplify the description of statistical variation of soil hydraulic properties. Peck [7] defined a scaling parameter α as being the ratio of the microscopic characteristic length of a soil and the characteristic length of a reference soil:

$$\alpha_{\mathbf{x}} = \frac{\lambda_{\mathbf{x}}}{\lambda^*} \tag{4.1}$$

where $\mathbf{x} = \mathbf{x}_0, \mathbf{x}_1, ..., \mathbf{x}_{m-1}$ is a set of locations. The application of scaling, however, can be extended by estimating scale factors relative to the degree of saturation, with the result that the assumption of identical porosities can be eliminated. Nevertheless, scaling should be restricted to soil locations having some reasonable morphological similarity. By this simplification, the pattern of spatial variability is described by set of scale factors , each of which relates the soil hydraulic properties at each location to a representative mean. Three scaling parameters may be used to define a linear model of the actual spatial variability in the soil hydraulic properties as follows [14] :

$$K(h) = \alpha_k K^*(h^*) \tag{4.2}$$

$$\theta(h) = \alpha_\theta \theta^*(h^*) \tag{4.3}$$

$$h = \alpha_h h^*$$

in which , for the most general case , α_θ, α_k, α_h are mutually independent scaling factors for the water content, the pressure head and the hydraulic conductivity, respectively. The functions $K^*(h^*)$ and $\theta^*(h^*)$ representing scaled mean hydraulic conductivity and scaled mean water retention curves are described by well - known van Genuchten[12] model :

$$\theta^*(h^*) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{(1+|ah^*|^n)^m} & h^* < 0 \\ \theta_s & h^* \geq 0 \end{cases} \tag{4.4}$$

$$m = 1 - \frac{1}{n} \qquad n > 1 \tag{4.5}$$

$$K^*(h^*) = \begin{cases} K_s K_r^*(h^*) & h^* < 0 \\ K_s & h^* \geq 0 \end{cases} \tag{4.6}$$

where

$$K_r^*(h^*) = S_e^{*\frac{1}{2}} \left[1 - \left(1 - S_e^{*\frac{1}{m}}\right)^m\right]^2 \tag{4.7}$$

and

$$S_e^* = \frac{\theta^*(h^*) - \theta_r}{\theta_s - \theta_r} \tag{4.8}$$

in which h^* is scaled mean pressure head , θ_s and θ_r denote residual and saturated water contents, respectively, and K_s is the saturated hydraulic

conductivity. Equations 4.4 and 4.6 constitute a 5 - parameter model ($a, n, \theta_s, \theta_r, K_s$).

Less general scaling methods arise by invoking certain relationships between , α_θ, α_k and α_h. For example, the original Miller and Miller scaling procedure is obtained by assuming $\alpha_\theta = 1$ and $\alpha_h = \frac{1}{\sqrt{\alpha_k}}$. So in this case, actually knowledge about scaling factor for hydraulic conductivity suffices to fully describe spatial variability in the soil hydraulic properties (Equation4.2) as related to the mean characteristics.

The spatial variability may then be modelled by the scale factor random field given by the covariance structure (if the assumptions from Section 2.2.3 hold) . Theoretically [?], it is known that the logarithm of the scaling factor :

$$\alpha_{k\,\log} = \log\left(\alpha_k\right) \tag{4.9}$$

is normally distributed with:

$$\begin{aligned} E\left[\alpha_{k\,\log}\right] &= \mu_{\alpha_{k\,\log}} \\ Var\left[\alpha_{k\,\log}\right] &= \sigma^2_{\alpha_{k\,\log}} \end{aligned} \tag{4.10}$$

so the common approach, that is also used in our study, is to simulate $\alpha_{k\,\log}$ fields .

4.1.2 Data from Hupselse Beek watershed

To generate realizations of the scaling factor random field we used information about probability distribution and dependency structure estimated by Hopmans at al. [3] in the study area Hupselse Beek. All the data utilized in this project concern A - horizon when all 3 sampling schemes were combined. Figure 4.1 shows non-parametric form of semivariogram estimated for A and BC horizons. From that dependency range (R) and sill value ($\sigma^2_{\alpha_{k\,\log}}$) were taken to be : 5 m and 0.47 respectively. The mean value ($\mu_{\alpha_{k\,\log}}$) was specified as -0.1154.

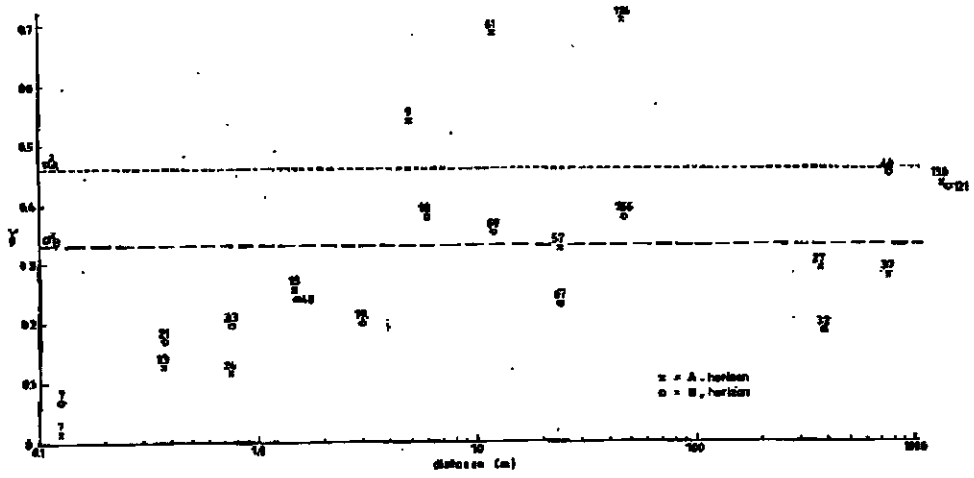

Figure 4.1: Semivariograms of scale factor values of A and BC horizons

4.2 Monte Carlo analysis

4.2.1 Classical approach

A classical way of doing Monte Carlo analysis in the case of deterministic models is to generate a great number of input field realizations with correct probabilistic behavior, present them to the model and deduce from all generated outputs their particular statistics (we were especially interested in the covariance structure of the output). This can be seen in Fig.4.2. Firstly, one has to provide a Gaussian random field generator with information about the spatial mean and variance - covariance structure. The information is usually obtained from experimental semi-variogram. Secondly, the model is excited for several times by different realizations of the Gaussian field . Lastly, all the output fields that correspond to the input realizations are analyzed in terms of first and second order moments . To gain an insight into controllability of the output variables by spatial variability of soil parameters (input fields), first and second order statistics are compared and usually functional relationship between them is derived.

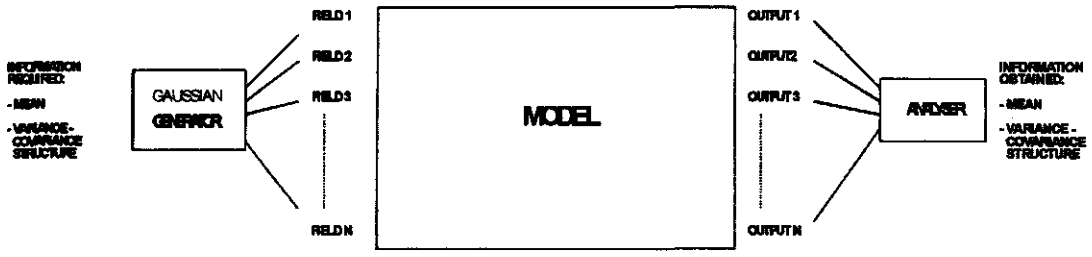

Figure 4.2: Monte Carlo analysis scheme

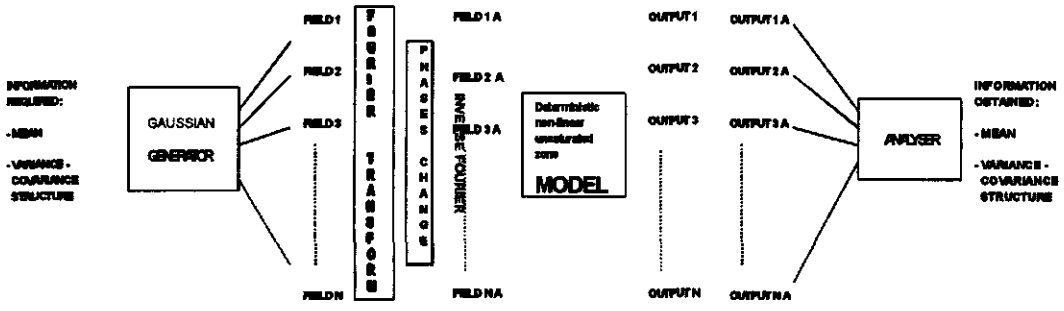

Figure 4.3: Novell aprroach to the classical Monte Carlo analysis

4.2.2 Modification - novel sensitivity analysis.

From the theoretical point of view , however, it is obvious that if the deterministic model is non-linear (and unsaturated zone models are non-linear) the second order statistics of the output do not only depend on second order properties of the input. Non - second order properties might be emphasized by non-linear model, so the standard Gaussian input field generation procedure cannot be used alone to detect this effect. As an alternative for the Gaussian method, we proposed a simple modification. We applied Fourier transform to the input fields, changed the phases of the transforms, and eventually took inverse transform to go back to space domain.

So finally we had two sets of input fields : first one generated according to classical Gaussian procedure and a second one generated by altering the phases of the Fourier transforms of the first set. It is worth to be stressed that, as proved by Equation 3.10 , the covariance structure of the second

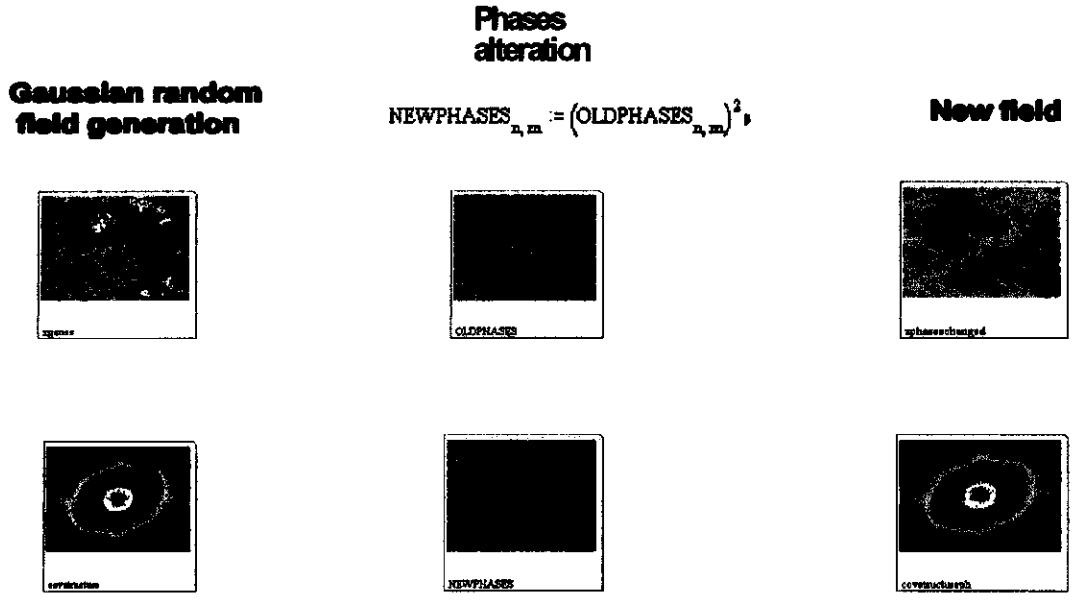

Figure 4.4: An example of phases altered Gaussian random field

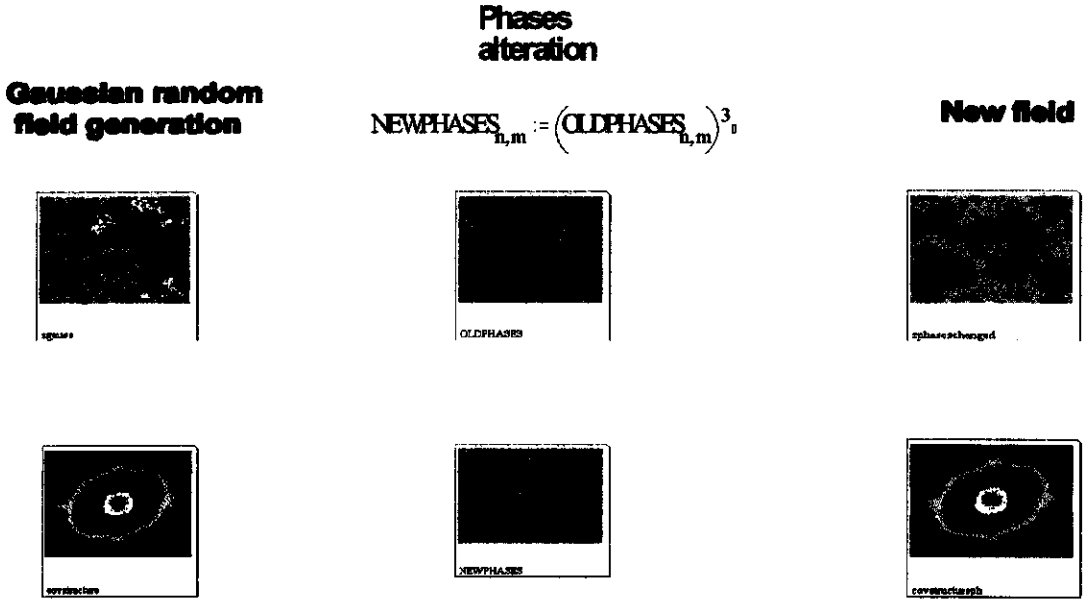

Figure 4.5: Another example of phases alteration : cubic transformation

input set is *exactly the same* as covariance structure of the first set. As illustrated in Fig. 4.3 the model was excited by the two input sets and , as a consequence, two output sets were obtained. We expected that covariance structure of the first output set *would be different* from the covariance structure of the second output set. Figure 4.4 clearly demonstrates a concept of phases alteration. In this example phases of the Gaussian field were squared and after taking inverse Fourier transform a new field was generated. Obviously, this is not the only way to change the phases. There are infinitely many possibilities, bearing in mind that we deal with *real* (according to the assumptions made in Section 2.2.3) random fields which imposes some constraints on the phases alteration function used, e.g., logarithmic phases transformation is not allowed since the phases of a Gaussian field are uniformly distributed over the range $[-\pi;\pi]$. In Fig.4.5 cubic transformation of the Gaussian filed phases was performed. One can easily observe the difference between the "new fields " from Fig. 4.5 and Fig.4.4. In contrast, their covariance structures are exactly the same. Therefore, by altering the phases of just one realization of the Gaussian field in almost arbitrary way many different realizations might be produced.

4.3 Random field simulation by convolution

Realizations of the scaling factor for hydraulic conductivity random field that follows the assumptions mentioned in Section 2.2.3 were simulated using a new spectral modification of simple nearest - neighbors model [1]. According to notation introduced in Section 3 the field $\{\mathbf{Z}(\mathbf{x})\}$ [2] will be denoted as $\mathbf{Z}(n,m)$. We assumed that the $\mathbf{Z}(n,m)$ was determined by the classical nearest - neighbour model:

$$\mathbf{Z}(n,m) = \sum_{n_1,m_1} d(n-n_1, m-m_1)\varepsilon(n_1,m_1) \tag{4.11}$$

where:

[1] Description of nearest-neigbors model that was, in combination with Monte Carlo analysis , applied to analyse the stochastic nature of output variables of 1-D unsaturated zone model can be found in Anderson and Shapiro [1]

[2] The scaling factor for hydraulic conductivity random field should be notified as $\{\alpha_{k\,\log}(\mathbf{x})\}$, but since the simulation method described in this Section might be apllied to generate the fields of the other spatial variables , the general notation was used.

$$
\begin{aligned}
n, m, n_1, m_1 &= 0, ..., 2^b - 1 \\
b &= \text{positive integer that describes discretization density}
\end{aligned}
$$

$$
d(\nu, \kappa) = \begin{cases} 1 \;\; if \;\; (2^{b-1} - \nu)^2 + (2^{b-1} - \kappa)^2 \leq R^2 \\ 0 \;\; if \;\; (2^{b-1} - \nu)^2 + (2^{b-1} - \kappa)^2 > R^2 \end{cases}
$$

R – dependency range evaluated from experiental semi-variogram

ε - Gaussian white noise matrix

$$
\begin{aligned}
E\left[\varepsilon(n_1, m_1)\right] &= 0 \\
Var\left[\varepsilon(n_1, m_1)\right] &= 1 \\
Cov\left[\varepsilon(n_1, m_1), \varepsilon(n_2, m_2)\right] &= 0
\end{aligned}
$$

Equation 4.11 shows that value of the field $\mathbf{Z}(n, m)$ at a particular location (n, m) is a sum of all neighbors $\varepsilon(n_1, m_1)$ that lie within a range R from the location. Although constant term 2^{b-1} was added for purely numerical reasons, the general idea of the $\mathbf{Z}(n, m)$ model remains the same.

Applying the discrete Fourier transform operator to the both sides of the Equation 4.11 we obtain:

$$
\mathcal{F}(\mathbf{Z}(n, m)) = \mathcal{F}(\sum_{n_1, m_1} d(n - n_1, m - m_1)\varepsilon(n_1, m_1)) \tag{4.12}
$$

The right hand side of the Equation 4.12 is nothing else than Fourier transform of a discrete convolution and can be rewritten as:

$$
\begin{aligned}
& \mathcal{F}(\sum_{n_1, m_1} d(n - n_1; m - m_1)\varepsilon(n_1, m_1)) \\
= \;\; & \mathcal{F}(d \star \varepsilon(n_1, m_1))
\end{aligned} \tag{4.13}
$$

with a property that:

$$
\mathcal{F}(d \star \varepsilon(n_1, m_1)) = \mathcal{F}(d(n, m))\mathcal{F}(\varepsilon(n, m)) \tag{4.14}
$$

Consequently, the $\mathbf{Z}(n, m)$ can be compactly expressed as:

$$
\mathbf{Z}(n, m) = \mathcal{F}^{-1}(\mathcal{F}(d(n, m))\mathcal{F}(\varepsilon(n, m))) \tag{4.15}
$$

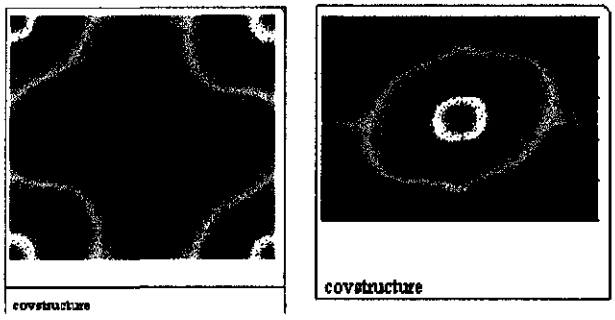

Figure 4.6: Covariance structure "without " and "with " multiplier $e^{\pi i(n+m)}$.

It is apparent that by means of $d(n,m)$ kernel function we can model any arbitrary covariance structure . In this project, however, we did not assume a particular parametric model of the covariance structure. To obtain a realization of the $\mathbf{Z}(n,m)$, denoted as $z(n,m)$, R parameter was taken from an experimental semivariogram (see Section 4.1.2) and a realization of the ε matrix, denoted as $\widetilde{\varepsilon}$,was generated . After standardizing the $z(n,m)$, the appropriate mean ($\mu_{\alpha_{k\log}}$) and sill ($\sigma^2_{\alpha_{k\log}}$) values were imposed. So our final realization $z(n,m)^*$of the $\mathbf{Z}(n,m)$ took the following form :

$$z^* = \left[\frac{z - E[z]}{\sqrt{VAR[z]}}\sqrt{\sigma^2_{\alpha_{k\log}}}\right] + \mu_{\alpha_{k\log}} \tag{4.16}$$

The covariance structure of the $z(n,m)^*$was calculated according to the formula:

$$b(\chi_0,\chi_1) = \mathcal{F}^{-1}\left(\left|\mathcal{F}\left(z(n,m)^* - \mu_\alpha\right)\right|^2 e^{\pi i(n+m)}\right) \tag{4.17}$$

where

$$\chi_0,\chi_1 = -2^{b-1}, 1-2^{b-1}, ..., 0, ..., 2^b - 1 - 2^{b-1}$$

The aim of introducing term $e^{\pi i(n+m)}$ to the Equation 4.17 was to present information about covariance structure, encoded in a power spectrum, in the most readable way (see Figure 4.6), i.e. in the middle of a picture.

Figure 4.7 gives an impression of typical realizations of the field and its covariance structure. The realizations of covariance structure in both cases match properties described in Section 2.2.1 except isotropy and thus

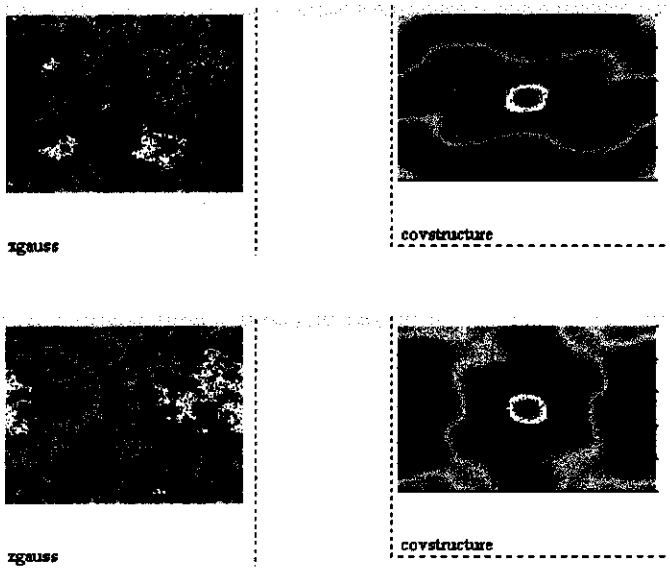

Figure 4.7: Two possible realizations of $z(n,m)$*and corresponding $b(\chi_0,\chi_1)$

quadrant symmetry. On the other hand , the underlying covariance structure $B(\chi_0,\chi_1)$ (derived from the whole ensemble of the realizations of the $\mathbf{Z}(n,m)$) is direction independent, i.e., isotropic. This is guaranteed by the Equation 4.11.

4.4 Input fields generation scheme

As it was mentioned in Section 4.1.2 the probability density function of the logarithm of the scaling factor ($\alpha_{k\,\log}$) is assumed to be Gaussian. Consequently, we used the convolution method to generate several realizations of the $\alpha_{k\,\log}(\mathbf{x})$ field . From this set one particular realization whose covariance structure was almost isotropic[3] was selected. From now on this realization will be called "mother " field . In the next step the Fourier transform of the "mother " field was taken and phases in the Fourier space were calculated.

[3] Coivariance structure of ensemble of realizations of our randoim field is isotropic - that is guaranteed by the structure of our model. However, practically we deal with sample realizations of the field and so with sample realizations of covariance structure. If one has a bad luck the covariance structure may look like the upper-right picture of Figure 4.7

Afterwards they were randomized five times using uniform pseudo-random number generator on the interval $[-\pi;\pi]$ to produce 5 input fields out of the mother field.

Remark 4 *This procedure is known as a classical spectral method for generating random fields. A realization $\alpha_{k\log}(\mathbf{x})$ of the random field with a given covariance function $B(\chi)$ (which in this case is the covariance function of the "mother " field) is generated by invoking the Wiener - Khinchine theorem (see Equation ??). As it was mentioned before the theorem states that the Fourier transform of the covariance function equals the spectrum $S(\omega)$ of the$\alpha_{k\log}(\mathbf{x})$, namely*

$$S(\omega) = \mathcal{F}[B(\chi)] \tag{4.18}$$

where the spectrum of $\alpha_{k\log}(\mathbf{x})$ is defined as $S(\omega) = |\alpha_{k\log}(\omega)|^2$ with

$$\alpha_{k\log}(\omega) = \mathcal{F}[B(\chi)]^{\frac{1}{2}} e^{i\phi(\omega)} \tag{4.19}$$

So to numerically simulate different realizations of $\alpha_{k\log}(\mathbf{x})$ in space domain one has to substitute phases $\phi(\omega)$ in the above formula by uniformly distributed random field Ω on the interval $[-\pi;\pi]$ and take the inverse Fourier transform which can be written as:

$$\alpha_{k\log}(\mathbf{x}) = \mathcal{F}^{-1}\left[\mathcal{F}[B(\chi)]^{\frac{1}{2}} e^{i\Omega}\right] \tag{4.20}$$

The random phases of the 5 input fields were then altered using simple sorting function. This operation indicated in Figure 4.8 by the arrow under the phases of the "mother " field picture , assigns the random phases to different frequencies without changing the values of the phases. Only is the phases location altered in the Fourier space. While it is true that the sorting is a "nasty " mathematical transformation since it is non - algebraic and a kind of periodicity is apparent in the fields produced that way (see reddish pictures in Figure 4.8), it was applied just to show problems that might occur with the classical Monte Carlo analysis. Once again it is important to stress that both input sets: one generated by the classical spectral method and the second one generated by sorting the phases of the first set, had exactly the same covariance structure as the "mother field ".

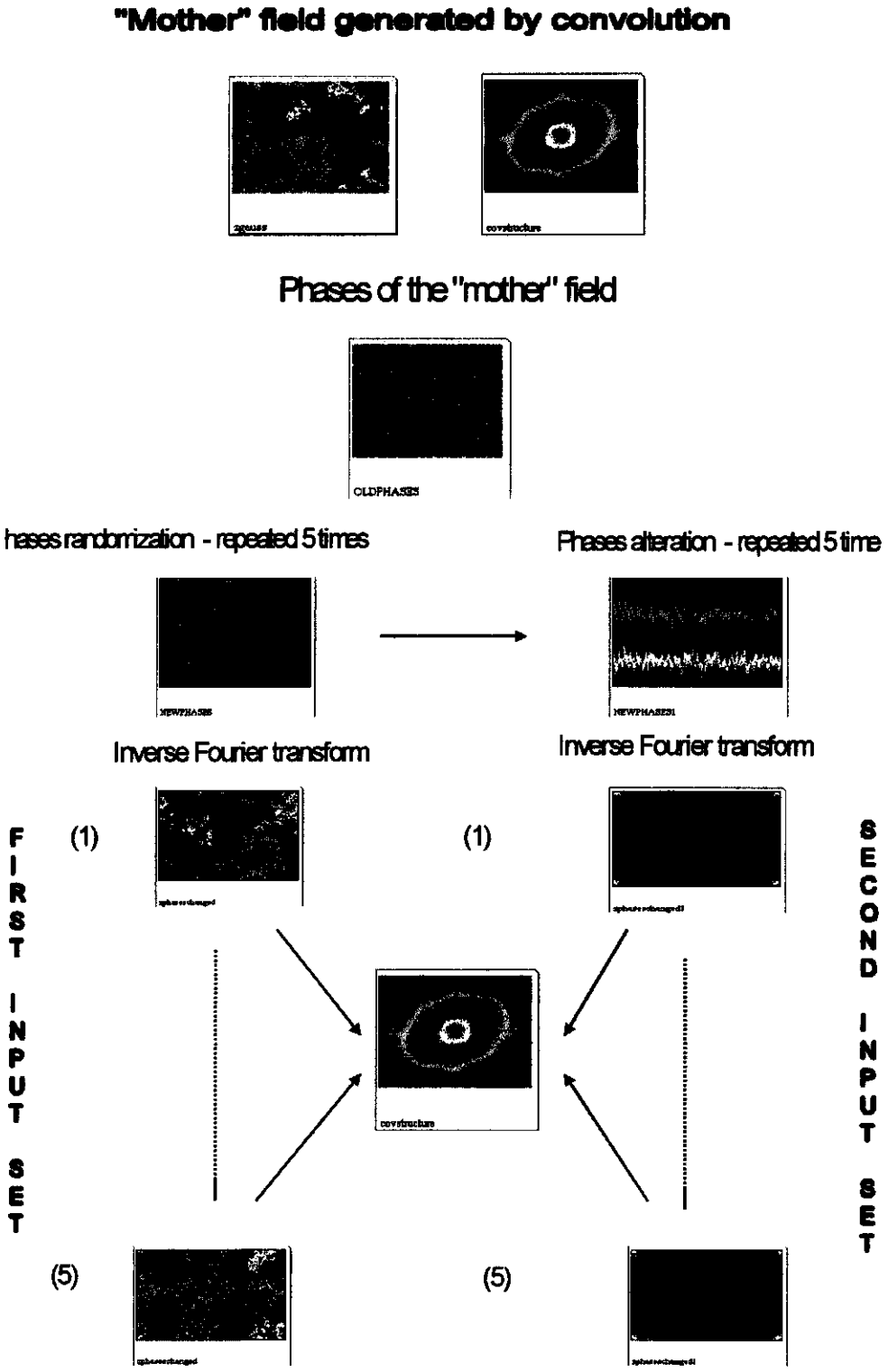

Figure 4.8: Input fields preparation scheme

4.5 Unsaturated zone water flow simulation

Vertical water flow through the column of loam was simulated with the finite element code HYDRUS 2-D ver.1.0 (Simunek at al [11]) We considered a two - dimensional region 10 m wide and 5 m deep, which was discretized on a 64x128 grid. At the upper boundary we assumed athmospheric water flow with maximum infiltration from 0,5h till 2.5h of a simulation time of 80 hours. At the lower boundary a free drainage occurred.. The vertical boundaries were impermeable. Initial pressure head was set to -100 cm. The model was excited by the two input sets described in the previous section. Figure 4.9 shows a summary of all the simulation parameters used in this study.

4.6 Examples of output fields analysis

Volumetric water content Θ was defined as an output variable from unsaturated zone model . To provide a rough description of the Θ spatial structure we estimated horizontal, band - limited autocorrelation function (HACF). Expression "band-limited " implies that the HACF was estimated only within the selected band, namely the submatrix (0-7 vertical grid units and 0-127 horizontal grid units) of the soil column. It was expected that in this near-surface zone the highest variation in the water content spatial distribution would occur, due to simulated rainfall event. HACF was calculated for three selected simulation times : 6h, 50h an 80h, using a well - known Fourier transform pair :

$$\begin{aligned} \rho_\theta(m) &= \mathcal{F}^{-1}\left(\frac{1}{N}\sum_{n=0}^{N-1}|\mathcal{F}(\theta_{n,m})|^2\right) \\ N &= 7 \\ m &= 0,1,..,127 \end{aligned} \tag{4.21}$$

Then, HACF of the Θ fields related to phases-randomized input set was compared with HACF of the Θ fields related to non-algebraically transformed input set. To get a better insight into differences between the two HACF's, we averaged each of them over the set of corresponding realizations of the Θ fields and presented them in the form of plot. In addition, for each simulation

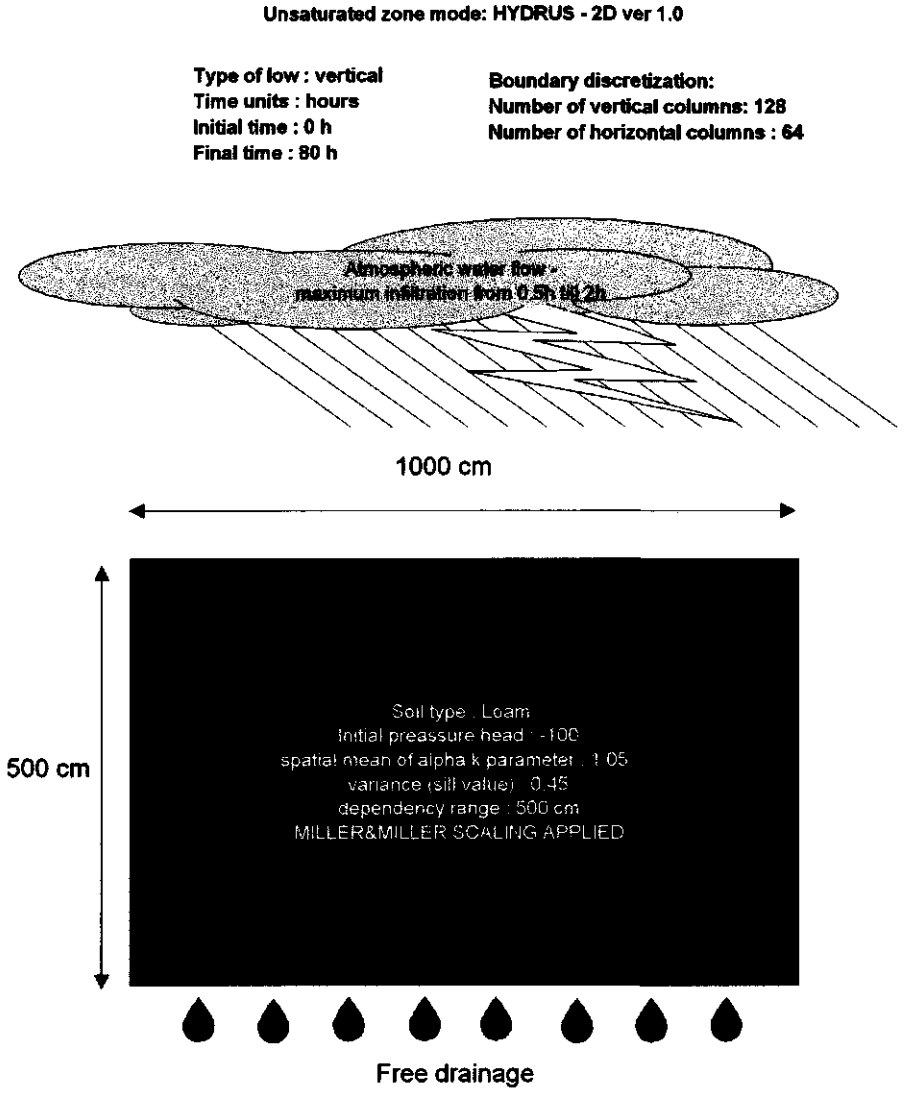

Figure 4.9: Parameters for water flow simulation

time and for each output set we estimated probability distribution function and accompanying second order moments.

Chapter 5

Results and Discussion

The HACF's of the Θ fields for two input sets are presented in Figure 5.1. By comparing the graphs it can be seen that were are differences between HACF's related to classically generated and phases - altered realizations of input fields. This effect is best illustrated by HACF's averaged over realizations of the Θ fields (see Figure 5.2). Table 5.1 illustrates second order moments associated with each realization. Systematic differences between means and variances of two sets of output fields were observed; means and variances of the second set were higher then corresponding moments from the first set. One may argue that differences in means were negligibly small, but taking into account magnitude of variances they were significant. Therefore, two sets of input fields with exactly the same covariance structure generated two sets of output fields with different variances, meaning that non-Gaussian effects were amplified by non-linear unsaturated zone model. In the analysis presented in this project we concentrated , however, on just two aspects of modified Monte Carlo analysis : means and variances. The idea was to show the maximum effect. Nevertheless many other aspects might have been considered, for example probability distribution peaks or moments of chosen fluxes etc.

		time =	6h	
realization nr	input set	1	input set	2
	mean	variance	mean	variance
1	0.317	$9.6 \cdot 10^{-4}$	0.329	0.001
2	0.32	$10 \cdot 10^{-4}$	0.328	0.001
3	0.316	$5.8 \cdot 10^{-4}$	0.333	0.001
4	0.315	$6.04 \cdot 10^{-4}$	0.329	0.001
5	0.321	$8.51 \cdot 10^{-4}$	0.334	0.001
average	0.318	$7.99 \cdot 10^{-4}$	0.33	0.001
		time =	50h	
realization nr	input set	1	input set	2
	mean	variance	mean	variance
1	0.273	$6.74 \cdot 10^{-4}$	0.293	$9.19 \cdot 10^{-4}$
2	0.281	$7.15 \cdot 10^{-4}$	0.287	$10 \cdot 10^{-4}$
3	0.275	$5.21 \cdot 10^{-4}$	0.299	$9.2 \cdot 10^{-4}$
4	0.271	$7.12 \cdot 10^{-4}$	0.292	$7.87 \cdot 10^{-4}$
5	0.288	$6.35 \cdot 10^{-4}$	0.299	$8.67 \cdot 10^{-4}$
average	0.277	$6.51 \cdot 10^{-4}$	0.294	$8.99 \cdot 10^{-4}$
		time =	80h	
realization nr	input set	1	input set	2
	mean	variance	mean	variance
1	0.271	$4.53 \cdot 10^{-4}$	0.293	$9.2 \cdot 10^{-4}$
2	0.279	$5.35 \cdot 10^{-4}$	0.285	$9.36 \cdot 10^{-4}$
3	0.272	$4.21 \cdot 10^{-4}$	0.296	$8.05 \cdot 10^{-4}$
4	0.269	$5.51 \cdot 10^{-4}$	0.289	$6.7 \cdot 10^{-4}$
5	0.286	$5.65 \cdot 10^{-4}$	0.297	$7.6 \cdot 10^{-4}$
average	0.275	$5.05 \cdot 10^{-4}$	0.292	$8.18 \cdot 10^{-4}$

Table 5.1: Second order moments of water content Θ in band - limited soil column domain for different simulation times for phases - randomized fields (input set 1) and non-algebraically phases transformed fields (input set 2)

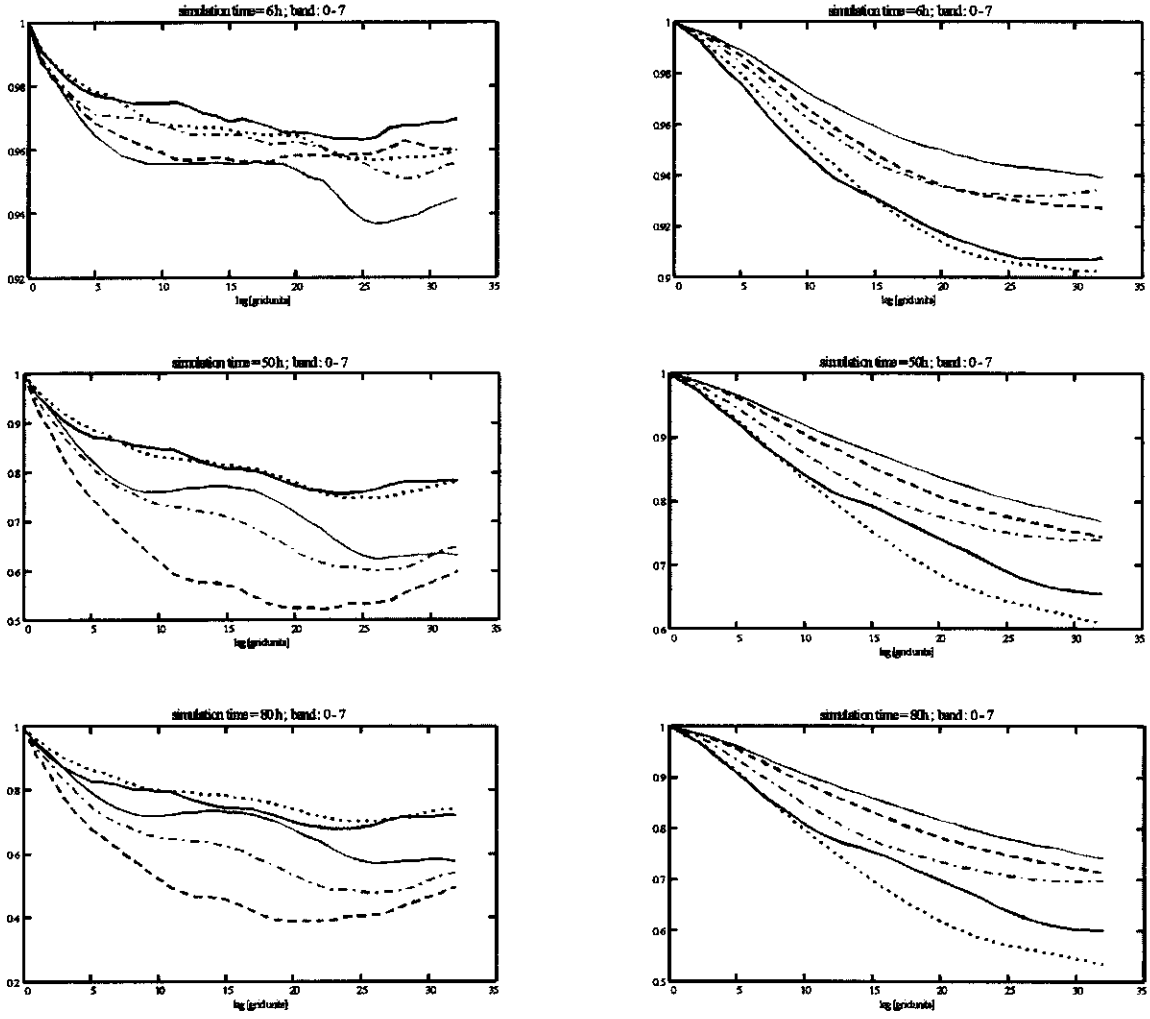

Figure 5.1: HACF of water content Θ in band - limited soil column domain for different simulation times for (left) phases - randomized input fields and (right) non-algebraically phases transformed input fields

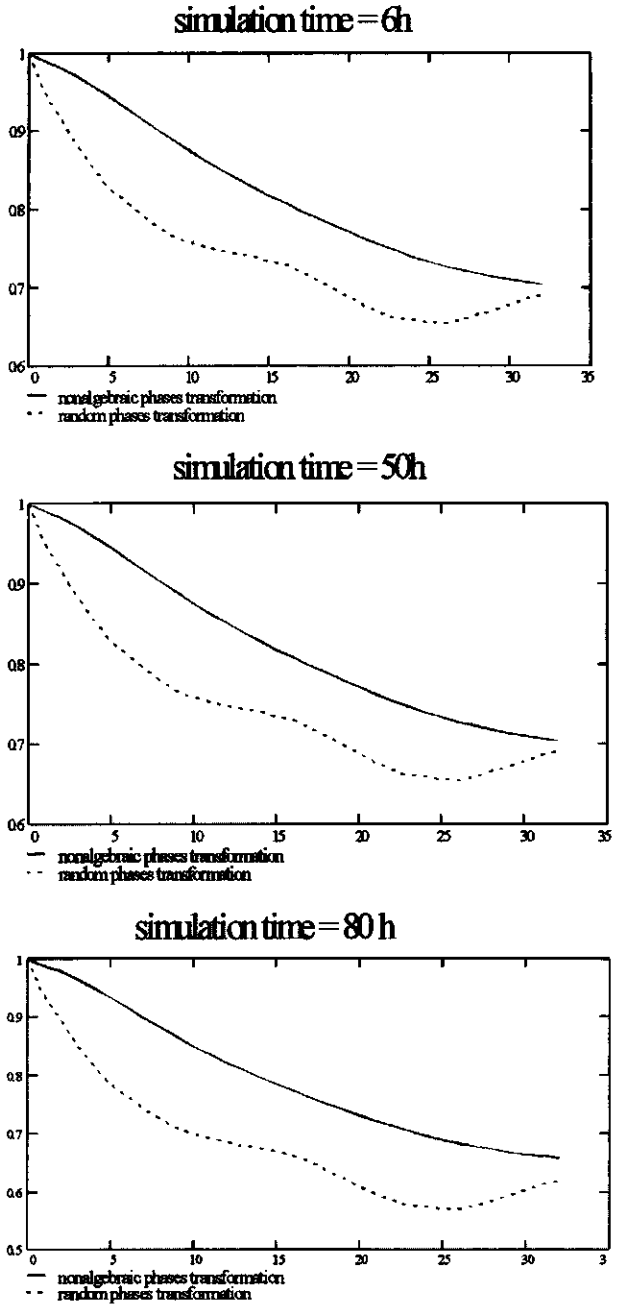

Figure 5.2: HACF averaged over realizations of two sets of Θ output fields

Chapter 6

Conclusions

In summary it can be stated that

1. Methodology developed in this project works and it is easy to implement
2. Non - Gaussian properties are important and should be taken into account especially in the case of non-linear models
3. The presented. tools should become an integral part of Monte Carlo analysis framework They can provide a user with an additional valuable information.

Bibliography

[1] Anderson, J. , and A. M. Shapiro (1983). Stochastic analysis of one dimensional steady state unsaturated flow : A comparison of Monte Carlo and perturbation methods. Water Resour. Res. 19(1): 121-133.

[2] Cislerova, M. (1987). Comparison of simulated water balance for ordinary and scaled soil hydraulic characteristics. Report Dept. of Water Resources, Wageningen Agricultural University

[3] Hopmans, J. W., and J. N. M. Stricker (1987) . Soil hydraulics properties in the study area Hupseelse Beek as obtained from three different scales of observations: An overview. Report nr 78 Dept. of Water Resources, Agricultural University Wageningen.

[4] Hopmans, J. W. , H. Schukking and P.J.J.F Torfs (1988) . Two-dimensional steady state unsaturated water flow in heterogeneous soils with autocorrelated soil hydraulics properties. Water Resour. Res. 24(12): 2005-2017.

[5] Jury, W. A. (1985). Spatial variability of soil physical parameters in solute migration: A critical literature review. Rep. EPRI EA-4228s. Electr. Power Res. Inst., Palo Alto, Calif.

[6] Miller, E. E., and R.D. Miller (1956). Physical Theory for cappilary flow phenomena. J. App. Physics 27(4): 324-332.

[7] Peck, A. J., R. J. Luxmoore, and J.L. Stolzy (1997). Effects of spatial variability of soil hydraulic properties in water budget modelling. Water Resour. Res. 15 (6) : 1543-1559.

[8] Priestley, M. B. (1981). Spectral analysis and time series. Academic Press, New York and London.

[9] Roth, K. (1995) Steady state flow in an unsaturated, two-dimensional macroscopically homogenuous, Miller-similar medium. Water Resour. Res. 33 (9): 2127-2140

[10] Russo, D. (1991) Stochastic analysis of simulated vadose zone solute transport in a vertical cross section of heterogenuous soil during non-steady infiltration. Water Resour. Res 27: 1361 - 1373.

[11] Simunek, J., M. Sejna, and M. Th. van Genuchten (1966). The HYDRUS 2-D software package for simulating water flow and solute transport in two-dimensional variably saturated media. U.S Salinity Labolatory, Agricultural Research Service, U.S Dept. of Agriculture, Riverside, California.

[12] van Genuchten, M. T. (1980). A closed form equation for predicting the hydraulic conductivity of unsaturated soils. Soil. Sci. Soc. Am. J. 44: 892-898.

[13] Vanmarcke, E. (1983). Random fields : Analysis and Synthesis. The MIT Press, Cambridge, Massachusetts, London.

[14] Vogel, T., M. Cislerova, and J.W. Hopmans (1991). Porous media with linearly variable hydraulic properties. Water Resour. Res. 27(10), 2735-2741.

Chapter 7

Appendix

7.1 Random fields generation in MathCad 6.0 plus

Radnom fields generation by spectral nearest-neigbours method was done by mean of MathCad 6.0 plus. A simple code was developed to generate unconditional scaling factor for hydraulic conductivity fields. Phases-change trick was implementend using built-in 2-D Fourier Transform functions. A characteristic example showing typical behaviour and computations to be performed, follows.

Nearest neighbour random field generation by convolution.

Rafal Wojcik, P.J.J.F Torfs

Field parameters input:

$IH := 10$ - length of the area in x-direction

$IV := 10$ - length of the area in z -direction

$b := 7$ - horizontal and vertical discretization parameter

$R := 5$ - range of dependency (from estimated semi - variogram)

$sill := 0.45$ - variance of the field (from estimated semi - variogram)

$mean_\alpha := 1.056$ - spatial mean

$k1 := 0 \quad k2 := 2^b \quad m := k1 .. k2 - 1$

$l1 := 0 \quad l2 := 2^b \quad n := l1 .. l2 - 1 \quad i := \sqrt{-1}$

Normally distributed pseudo - random number generator input:

$\mu := 0$ - mean

$\sigma := 1$ - standard deviation

$$d(n, m, R) := \begin{cases} 1 \text{ if } \left[\frac{(2^{b-1} - m)}{2^b} \cdot IH\right]^2 + \left[\frac{(2^{b-1} - n)}{2^b} \cdot IV\right]^2 \le R^2 \\ 0 \text{ otherwise} \end{cases}$$

{start of the random field generation by Fourier transform convolution}

$D_{n,m} := d(n, m, R)$

$N_n := mnorm(k2, \mu, \sigma)$

$$Normal(n) := \begin{cases} U \leftarrow N_0 \\ \text{for } i \in 1..n \\ \quad U \leftarrow augment(U, N_i) \\ U \end{cases}$$

{generation of normally distributed random matrix}

$\varepsilon := Normal(l2 - 1)$

$F_\varepsilon := CFFT(\varepsilon)$

$FD := CFFT(D)$

$Fz_{n,m} := F_{\varepsilon_{n,m}} \cdot FD_{n,m}$

{convolution}

$z := ICFFT(Fz)$

{inverse FFT of the convolution = Gaussian random field}

$$zgauss := \left[\left(\frac{z - mean(z)}{\sqrt{var(z)}}\right) \cdot \sqrt{sill}\right] + mean_\alpha$$

{imposing spatial mean and variance}

Phases - changed field generation:

$Fzgauss := CFFT(zgauss)$

$OLDPHASES_{n,m} := arg(Fzgauss_{n,m})$

$RAND_{n,m} := rnd(2 \cdot \pi) - \pi$

$NEWPHASES_{n,m} := (RAND_{n,m})$

{phases randomization procedure - small square on the right hand side says that it is excluded now}

$NEWPHASES1^{\langle n \rangle} := sort(NEWPHASES^{\langle n \rangle})$

{non-algebraic phases transformation - sorting all the columns of phases matrix in ascending order}

$A := NEWPHASES \quad A1 := NEWPHASES1$

Figure 7.1: MathCad code - Part1

Imposing symmetry on A and A1 matrices (technical step to assure correctness of inverse Fourier transform) :

$m := 1..2^{b-1}-1 \quad n := 1..2^{b-1}-1$

$A_{0,m} := -A_{0,2^b-m}$

$A_{2^{b-1},m} := -A_{2^{b-1},2^b-m}$

$A_{n,0} := -A_{2^b-n,0}$

$A_{n,2^{b-1}} := -A_{2^b-n,2^{b-1}}$

$s := 1..2^{b-1}-1 \qquad m := 1..2^{b-1}-1$

$A_{n,m} := -A_{2^b-n,2^b-m}$

$n := 1..2^{b-1}-1 \qquad m := 2^{b-1}+1..2^b-1$

$A_{n,m} := -A_{2^b-n,2^b-m}$

$A_{0,0} := OLDPHASES_{0,0}$

$A_{0,2^{b-1}} := OLDPHASES_{0,2^{b-1}}$

$A_{2^{b-1},0} := OLDPHASES_{2^{b-1},0}$

$A_{2^{b-1},2^{b-1}} := OLDPHASES_{2^{b-1},2^{b-1}}$

$m := 1..2^{b-1}-1 \quad n := 1..2^{b-1}-1$

$A1_{0,m} := -A1_{0,2^b-m}$

$A1_{2^{b-1},m} := -A1_{2^{b-1},2^b-m}$

$A1_{n,0} := -A1_{2^b-n,0}$

$A1_{n,2^{b-1}} := -A1_{2^b-n,2^{b-1}}$

$s := 1..2^{b-1}-1 \qquad m := 1..2^{b-1}-1$

$A1_{n,m} := -A1_{2^b-n,2^b-m}$

$n := 1..2^{b-1}-1 \qquad m := 2^{b-1}+1..2^b-$

$A1_{n,m} := -A1_{2^b-n,2^b-m}$

$A1_{0,0} := OLDPHASES_{0,0}$

$A1_{0,2^{b-1}} := OLDPHASES_{0,2^{b-1}}$

$A1_{2^{b-1},0} := OLDPHASES_{2^{b-1},0}$

$A1_{2^{b-1},2^{b-1}} := OLDPHASES_{2^{b-1},2^{b-1}}$

$n := 0..2^b-1 \qquad m := 0..2^b-1$

$NEWCFFT_{n,m} := \left(\left|Fzgauss_{n,m}\right|\right)\cdot e^{A_{n,m}\cdot i}$ {construction of a new Fourier transform out of the phases - changed Fzgauss transform}

zphaseschanged := ICFFT(NEWCFFT) {random field after phases change - Gaussian space}

$zphaseschangedlog_{n,m} := e^{\left(zphaseschanged_{n,m}\right)}$ {Exponential transformation to get rid of negative values of zphaseschanged field - Log space }

$NEWCFFT1_{n,m} := \left(\left|Fzgauss_{n,m}\right|\right)\cdot e^{A1_{n,m}\cdot i}$ {Procedure repeated for phases changed r.f}

zphaseschanged1 := ICFFT(NEWCFFT1)

$zphaseschangedlog1_{n,m} := e^{\left(zphaseschanged1_{n,m}\right)}$

{Writing the fiels to o the ASCII files}

WRITEPRN(f1) := Re(submatrix(zphaseschangedlog11, $2^{b-1}-1$, k1, k2- 1))

WRITEPRN(f1) := Re(submatrix(zphaseschangedlog111, $2^{b-1}-1$, k1, k2- 1))

Figure 7.2: MathCad code - Part 2