FORSCHUNGSZENTRUM ROSSENDORF

Archiv-Ex.:

FZR-243
Dezember 1998

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S. M. Prigarin[1], K. Noack

Abstract

Up-to-date methods of numerical modelling of random fields were applied to investigate some features of solute transport in saturated porous media with stochastic hydraulic conductivity. The paper describes numerical experiments which were performed and presents the first results.

1. Introduction

The analysis of mass transport in groundwater systems is very important in view of problems of environment pollution by chemical compounds and radionuclides. In addition to experimental investigations, mathematical modelling and numerical simulation of solute transport in porous media is of essential interest. Due to the complexity of the physical process, the uncertainty of hydrological parameters and the spatial variability in soil properties, the stochastic approach is extensively used (see, for example, [1-10]). This approach assumes some of the parameters of the governing equations to be realisations of random fields.

The goal of the present paper is to study the influence of randomness of hydraulic conductivity on the solute transport. The numerical experiments performed use two-dimensional flow models with stochastic fields of conductivity of the porous medium. To simulate the random fields we apply various numerical methods including new models that were elaborated in Novosibirsk Institute of Computational Mathematics and Mathematical Geophysics [11-13].

2. Governing equations and description of models

The transport of non-reactive dissolved solutes through saturated soil and aquifer materials can be described by the convection-dispersion equation

$$\frac{\partial(\theta C)}{\partial t} = div\,(\boldsymbol{D}\ \boldsymbol{grad}\ C) - div\,(\boldsymbol{U}C) + \Phi(\boldsymbol{x},t,C) \tag{1}$$

with

$$D_{ii} = (\alpha_L - \alpha_T)\frac{U_i^2}{|\boldsymbol{U}|} + \alpha_T|\boldsymbol{U}| + D^*,$$

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$$D_{ij} = (\alpha_L - \alpha_T)\frac{U_i U_j}{|\boldsymbol{U}|}, \quad i \neq j,$$

$$\boldsymbol{U} = -K \; \boldsymbol{grad} \; H$$

and the filtering equation (Darcy`s law)

$$\boldsymbol{div}(K \; \boldsymbol{grad} \; H) + Q = 0. \tag{2}$$

The quantities in these equations are:

C - solute concentration, defined as mass per volume of solution,

θ - volumetric water content in a porous medium (porosity),

$\boldsymbol{U}$ - vector of the fluid filtration velocity and $\boldsymbol{U}/\theta$ is the specific discharge (i.e. the pore water velocity),

Φ - source-sink term of solute,

$\boldsymbol{D}$ - dispersion tensor with coefficient of molecular diffusion D^* and with coefficients α_L, α_T in longitudinal and transverse direction, respectively,

K - hydraulic conductivity,

H - pressure head,

Q - source-sink term of water,

t - time variable and

$\boldsymbol{x}$ - spatial variable.

The rigorous derivation of the convection-dispersion equation from microscopic or molecular physical principles remains an open research problem [3]. Nevertheless, analytical and numerical solutions of this equation have been successfully used as models for a large number of experimental studies.

Remark 1. Equation (1) is used for unsaturated soil as well as for saturated. But in the case of partially saturated porous medium equation (2) is replaced by Richard's equation and some assumptions must be added on dependence between conductivity, pressure head and water saturation (see, for example, [3,5,8,10,14]).

Remark 2. Note that the general form of the dispersion tensor $\boldsymbol{D}$ is similar to the general representation of a spectral tensor for solenoidal isotropic random vector-valued fields [15].

Below, only the two-dimensional case, $\boldsymbol{x}=(x,y)$, without source-sink terms, $\Phi=Q=0$, is considered. Furthermore, it is assumed that the porosity θ is a constant and that the conductivity K is a realisation of a random field with lognormal one-dimensional distribution with parameters μ and σ,

$$K(x,y) = exp(\sigma\xi(x,y) + \mu). \tag{3}$$

$$\mathbf{E}\, K(x,y) = K_0 = exp(\sigma^2/2+\mu),$$

$$\mathbf{V}\, K(x,y) = S^2 = \left(exp(\sigma^2)-1\right)exp(\sigma^2+2\mu),$$

where **E** denotes the average value and **V** is the variance.

Autoregressive schemes and spectral methods were used to numerically construct the Gaussian field $\xi(x,y)$ with different correlations. For example, the homogeneous discrete Gaussian field $\xi(i\,\Delta x,\, j\,\Delta y) = \eta(i,j)$ with the correlation function

$$\mathbf{E}\, \xi(i\,\Delta x,\, j\,\Delta y)\, \xi(0,\, 0) = \rho_x^{i\Delta x}\, \rho_y^{j\Delta y}, \qquad \rho_x,\, \rho_y \in (0,1), \tag{4}$$

$$\mathbf{E}\, \eta(i,j)\, \eta(0,0) = a^i\, b^j, \qquad a=\rho_x^{\Delta x},\ b=\rho_y^{\Delta y}$$

can be simulated according to the autoregressive scheme:

$$\eta(0,0) = \varepsilon(0,0),$$

$$\eta(i,0) = a\,\eta(i\text{-}1,0) + (1-a^2)^{1/2}\,\varepsilon(i,0), \qquad i>0,$$

$$\eta(0,j) = b\,\eta(0,j\text{-}1) + (1-b^2)^{1/2}\,\varepsilon(0,j), \qquad j>0,$$

$$\eta(i,j) = a\,\eta(i\text{-}1,j) + b\,\eta(i,j\text{-}1) - a\,b\,\eta(i\text{-}1,j\text{-}1) + (1-a^2-b^2+a^2\,b^2)^{1/2}\,\varepsilon(i,j), \quad i,j>0,$$

where ρ_x and ρ_y are parameters of the correlation function, Δx and Δy are the steps in x and y directions, respectively, $\varepsilon(i,j)$ are independent normal variables with zero mean and unit variance. The so-called spectral models were used to simulate homogeneous isotropic Gaussian random fields with the correlation functions

$$\mathbf{E}\, \xi(x,y)\, \xi(0,0) = B(r), \qquad r=(x^2+y^2)^{1/2},$$

where

$$B(r) = \frac{sin(\lambda r)}{\lambda r}, \tag{5}$$

$$B(r) = exp(-\lambda r), \tag{6}$$

$$B(r) = J_0(\lambda r), \tag{7}$$

and J_0 is the Bessel function of the first kind (see, [11-13] and Appendix).

Remark 3. Correlation function of the Gaussian field $\xi(x,y)$ and covariances of the random field of conductivity $K(x,y)$ in Eq. (3) are connected by the following relation (see, for example [13])

$$Cov_K(x,y) = S^2 \frac{exp(\sigma^2 Cov_\xi(x,y)) - 1}{exp(\sigma^2) - 1} + K_0^2$$

where

$$Cov_K(x,y) = \mathbf{E}\, K(x,y)\, K(0,0), \qquad Cov_\xi(x,y) = \mathbf{E}\, \xi(x,y)\, \xi(0,0).$$

For the analysis presented here the following boundary value problems are considered (see Fig. 1): The flow region is assumed to be a rectangular with zero-flux left and right boundaries; a pressure head H_0 is fixed at the lower boundary and the water entry is located at the upper boundary where a pressure head H_1 ($H_1 > H_0$) is determined (Problem A) or a steady, spatially constant influx is fixed (Problem B). The flow region is assumed to be free of pollution at the initial moment of time. The pollution (with unit concentration) comes with the water flow either through a central part of the upper boundary or through the entire width of the water entry.

Problem A: upper boundary with a fixed pressure head H_1 ($H_1 > H_0$)

Problem B: upper boundary with a fixed steady, spatial invariant influx

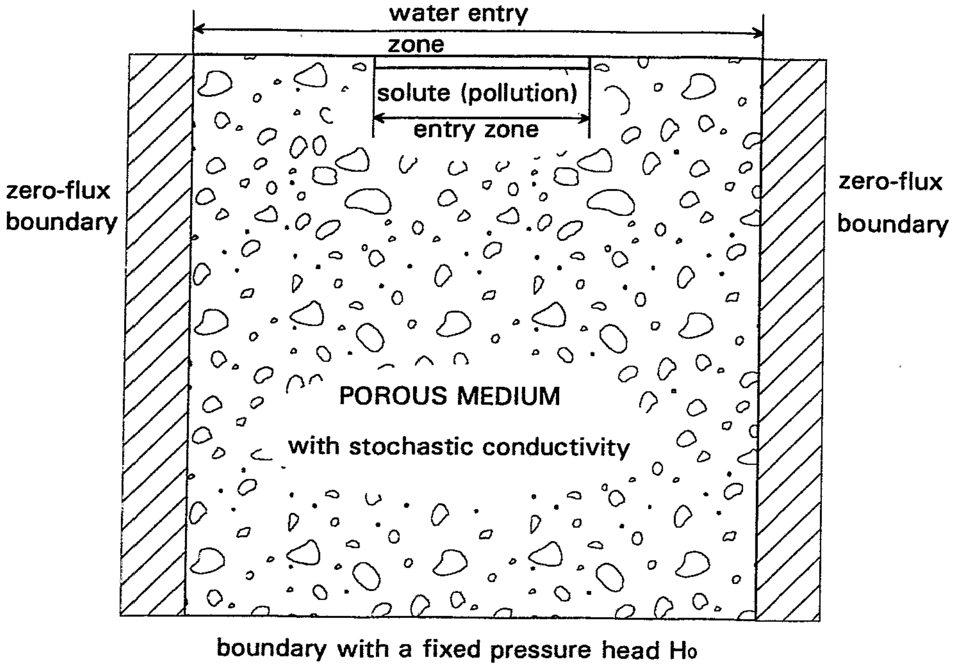


Fig. 1: Scheme of computational problems

3. Results of simulations

At the first stage of research the investigations were restricted to the dispersion-free pollution transport that is described by equation (1) with $D=0$. The following effects caused by randomness of the field of conductivity were observed in numerical experiments performed so far.

A) Essential increase of the polluted region in the medium

Figs. 2-6 represent some realisations of stochastic fields of logarithm of hydraulic conductivity, the correspondent fields of the pressure head and the asymptotic limit of pollution concentration, i.e. the values of $C(x,y,t)$ when $t \to \infty$. The problem A was solved for a 100×100 rectangular domain with the following parameters: $H_0=0$, $H_1=15$, $K_0=1$, $S^2=3.0$. The polluted area is much larger for stochastic fields of conductivity compared with the nonrandom case which is shown in Fig. 7. This increase of the pollution area is of essential interest if the contamination is important even for small values of concentration.

B) Decrease of the breakthrough time and smoothing of the pollution front (a variant of Problem B)

An example for the temporal behaviour of the polluted region in a medium with stochastic conductivity for such a boundary value problem is shown in Fig. 8 for a pollution entry zone which coincides with the whole upper boundary. A time diagram of the solute outflow at the lower boundary in a nonrandom medium has a step form as shown by the dashed line in Fig. 9 where t_0 is the breakthrough time. The solid line shows the outflow for the stochastic medium characterised by the same expectation value of conductivity. In the stochastic medium the step is smoothed and the breakthrough time t_s is smaller than t_0. The results presented in Figs. 8 and 9 correspond to the boundary value problem with hydraulic conductivity simulated according to model (3), (5) in a 100×100 rectangular domain with parameters $\lambda=0.5$, $H_0=0$, $Q=0.1$, $K_0=1$, $S^2=0.3$, $\theta=0.3$.

C) Decrease of the medium conductivity in average (Problem A)

In accordance with the filtering equation (2) for Problem A the integral water flux F through the medium is given by

$$F = \int_0^Y \frac{\partial H(x,y)}{\partial x} K(x,y)\big|_{x=0}\, dy = \int_0^Y \frac{\partial H(x,y)}{\partial x} K(x,y)\big|_{x=X}\, dy \qquad (8)$$

where $\{x=0,\ y\in(0,Y)\}$, $\{x=X,\ y\in(0,Y)\}$ are the sets of points of the lower and upper boundaries, respectively. For spatially invariant hydraulic conductivity $K(x,y)=K_0$ we have $F=F_0$, with

$$F_0 = (H_1 - H_0)K_0 Y / X. \qquad (9)$$

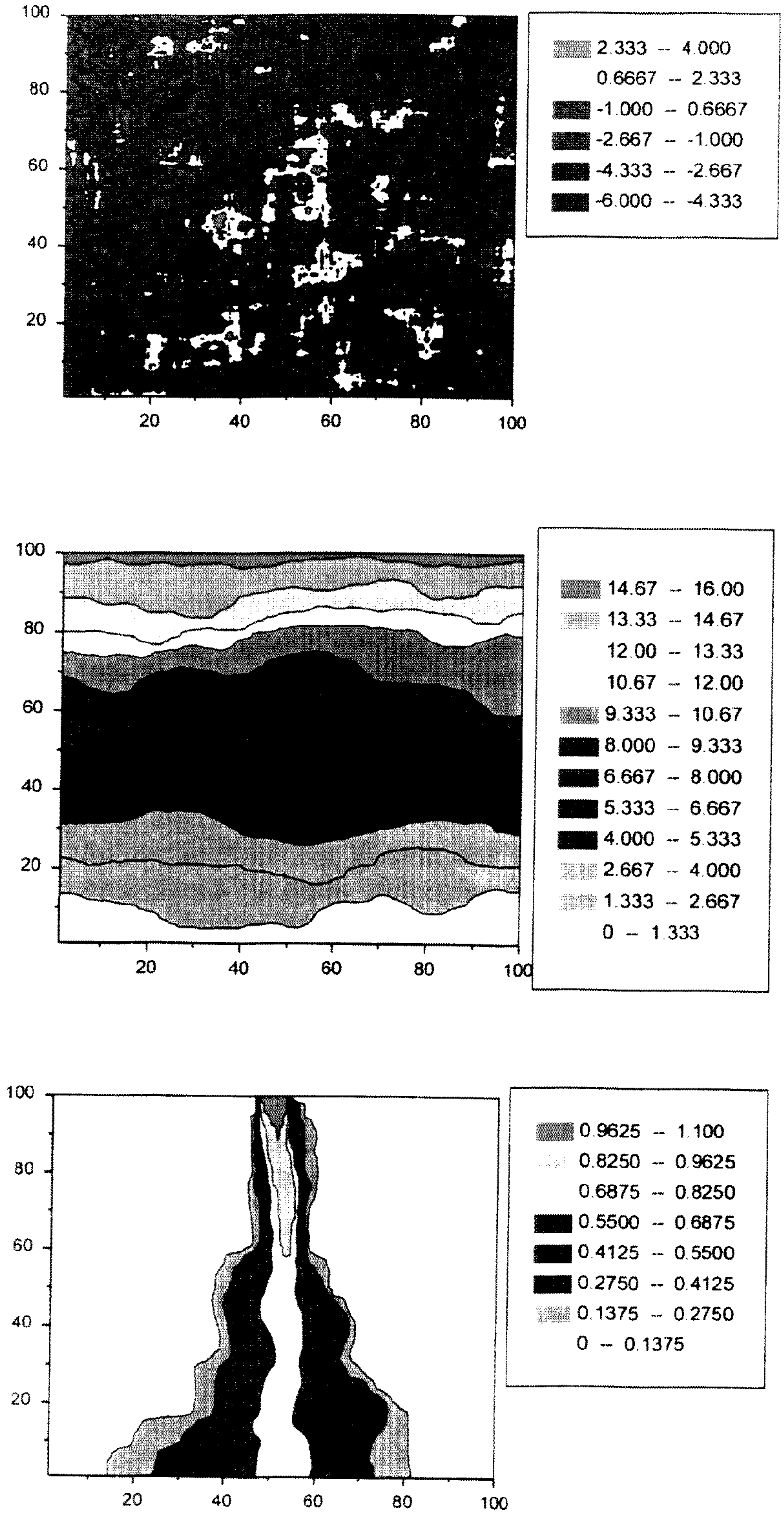


Fig. 2: Realisations of the fields of hydraulic conductivity, correspondent pressure head and asymtotic limit of concentration of pollution (from top to bottom) for Problem A, model (3) with correlation function (4).

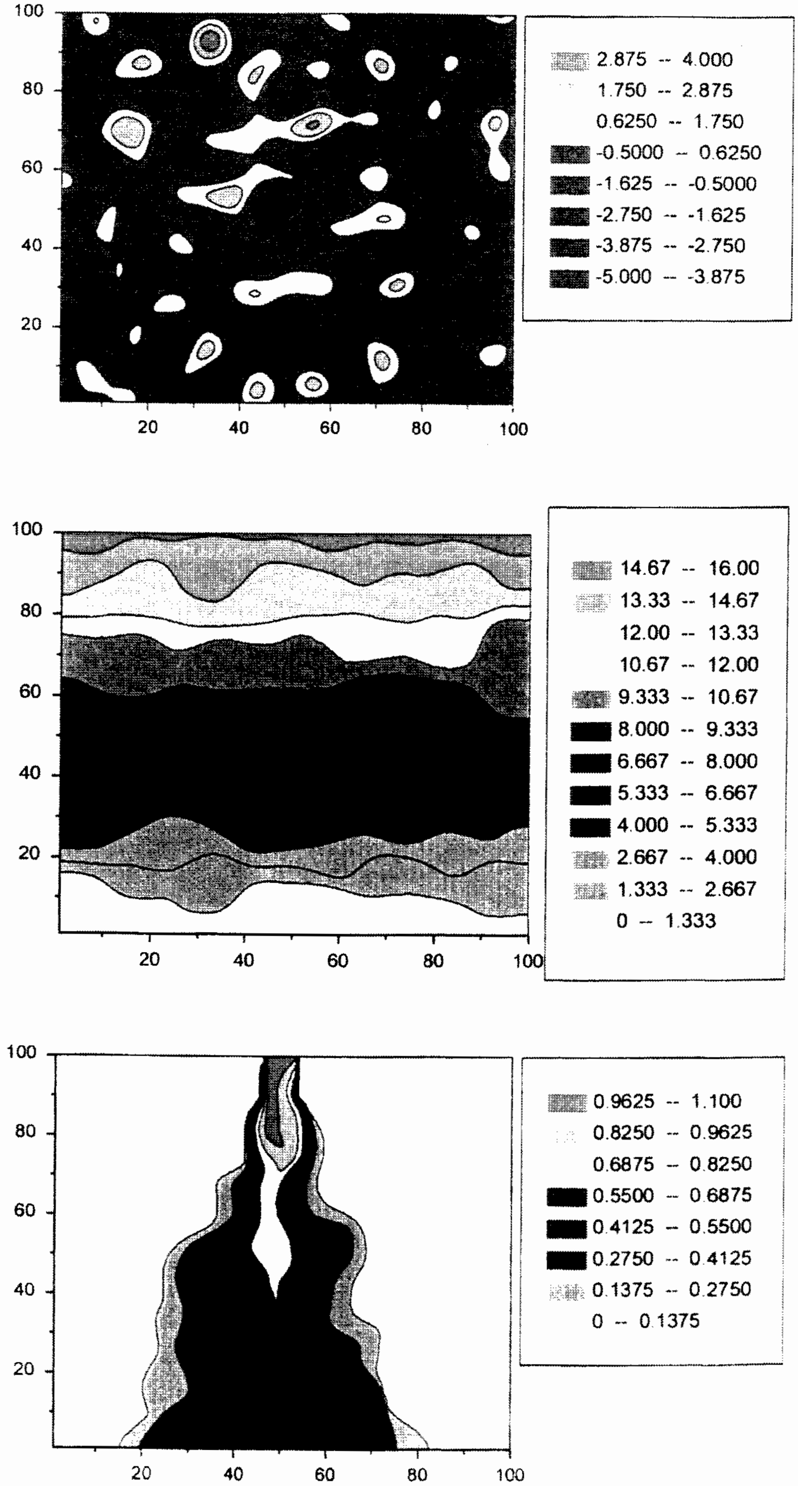


Fig. 3: Realisations of the fields of logarithm of hydraulic conductivity, correspondent pressure head and asymptotic limit of concentration of pollution (from top to bottom) for Problem A, model (3) with correlation function (5).

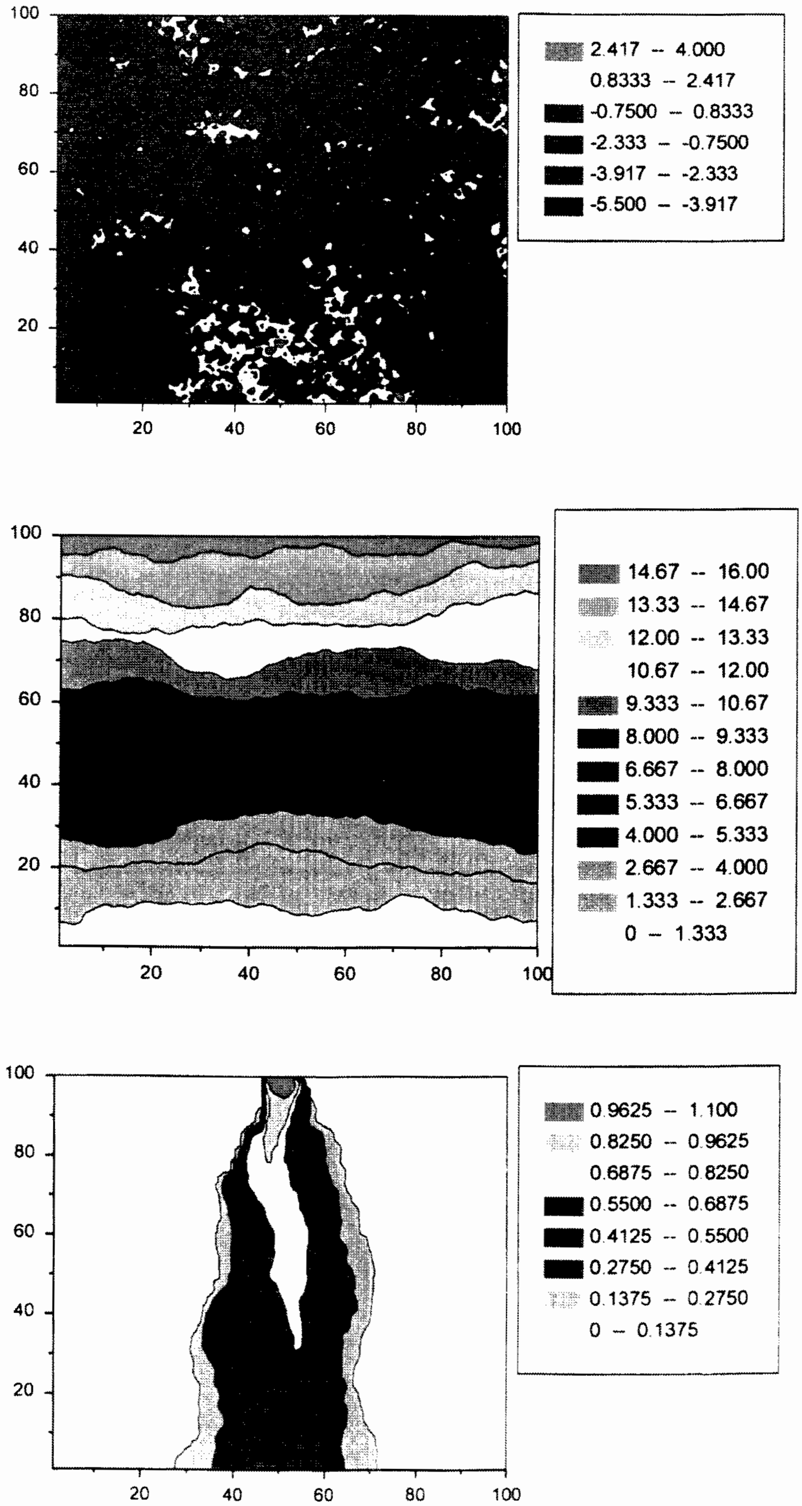


Fig. 4: Realisations of the fields of logarithm of hydraulic conductivity, correspondent pressure head and asymptotic limit of concentration of pollution (from top to bottom) for Problem A, model (3) with correlation function (6).

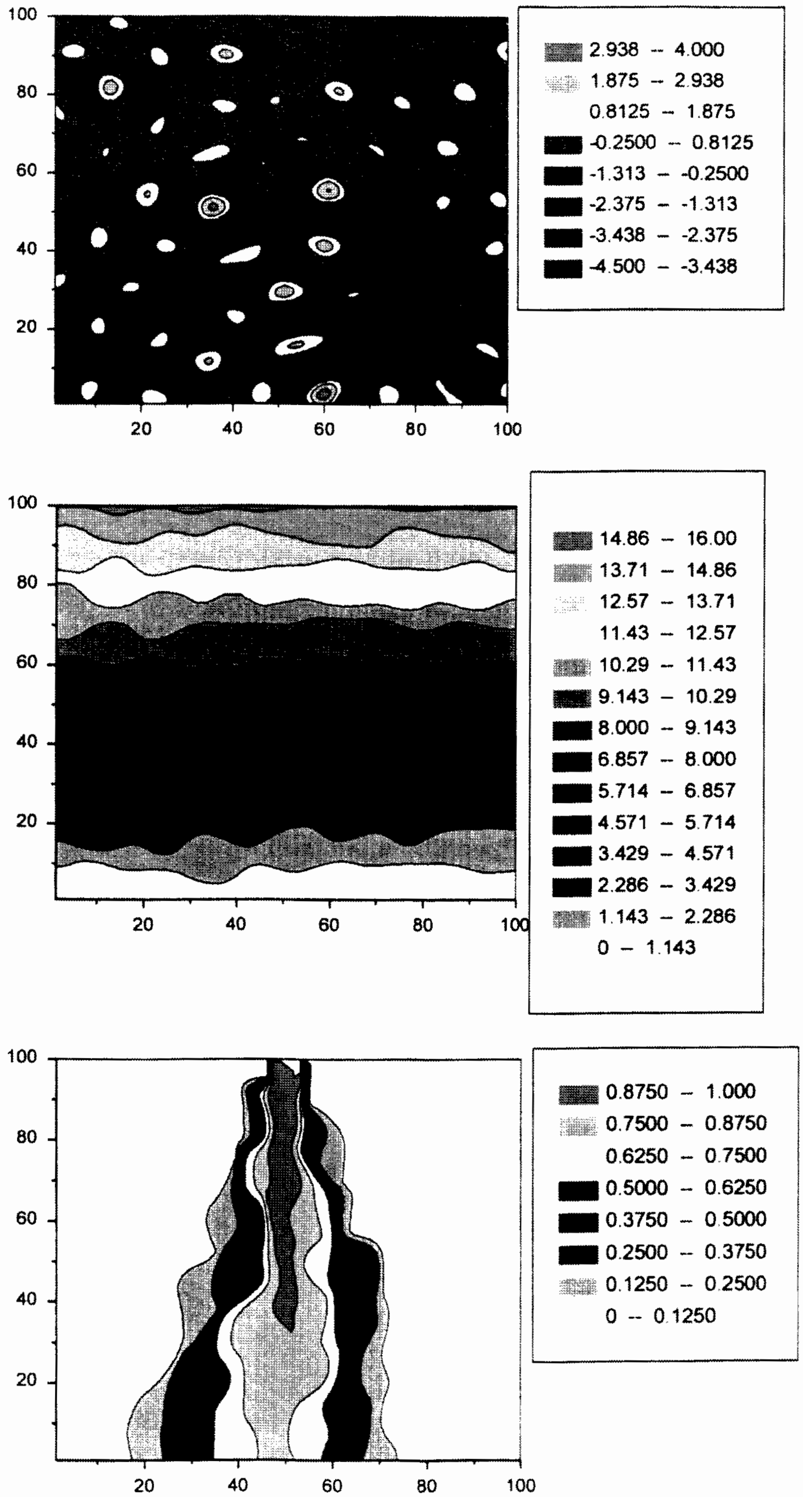


Fig. 5: Realisations of the fields of logarithm of hydraulic conductivity, correspondent pressure head and asymptotic limit of concentration of pollution (from top to bottom) for Problem A, model (3) with correlation function (7).

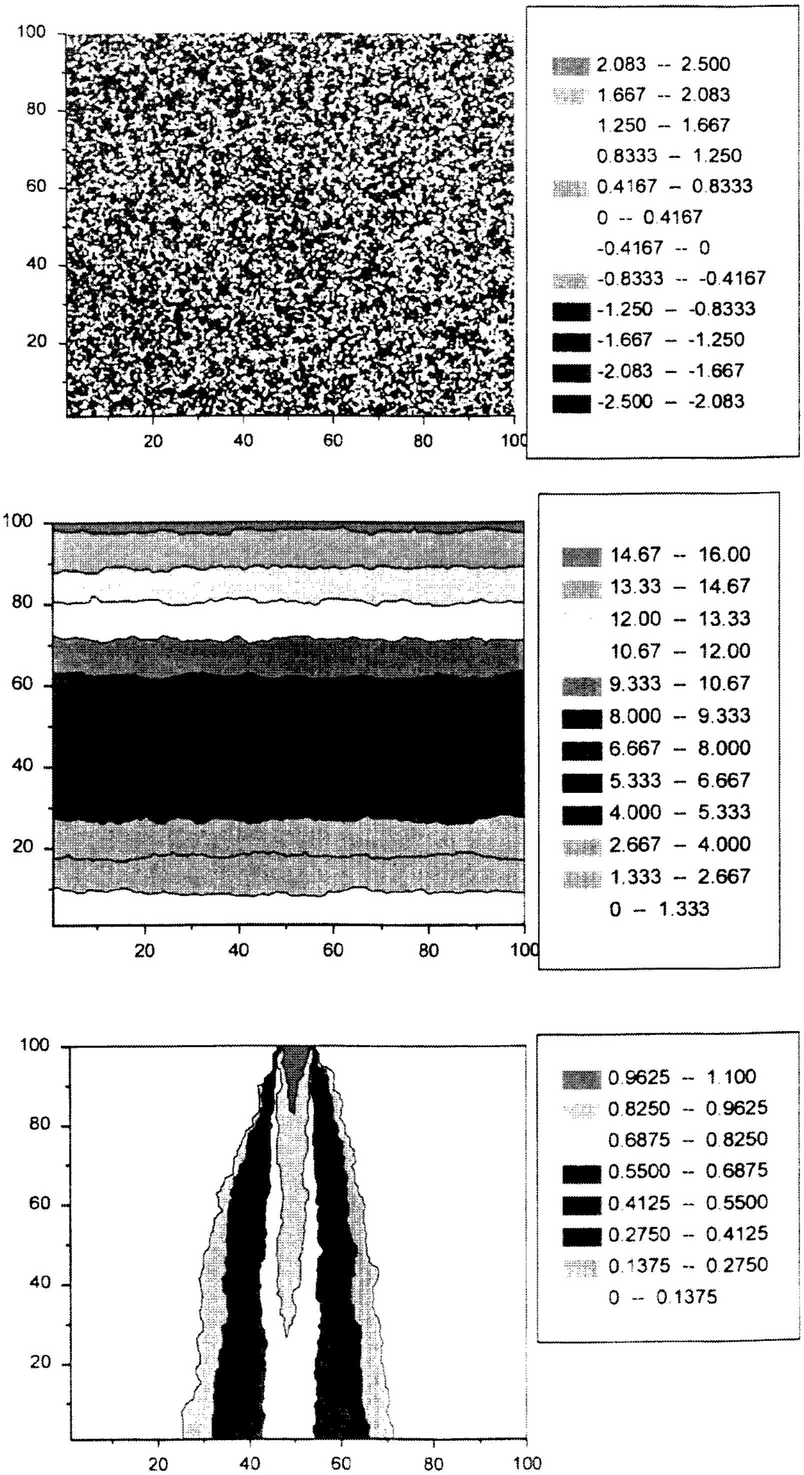


Fig. 6: Realisations of the fields of logarithm of hydraulic conductivity, correspondent pressure head and asymptotic limit of concentration of pollution (from top to bottom) for Problem A, model (3) with the Gaussian white noise as the random field ξ.

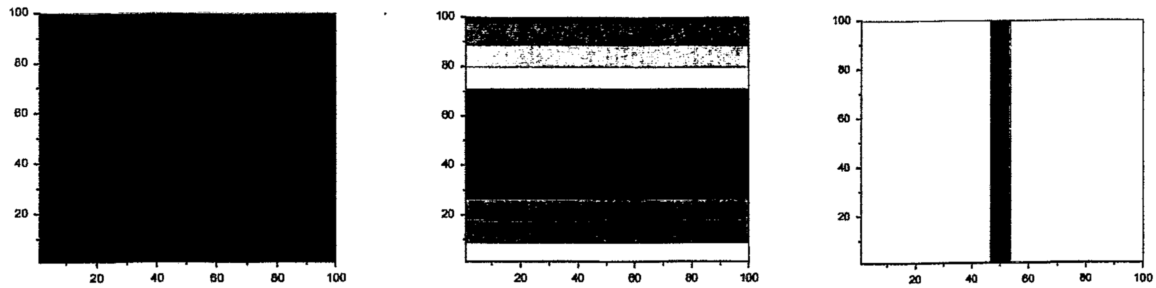


Fig. 7: Illustration concerning Problems A and B for spatially invariant (nonrandom) conductivity.

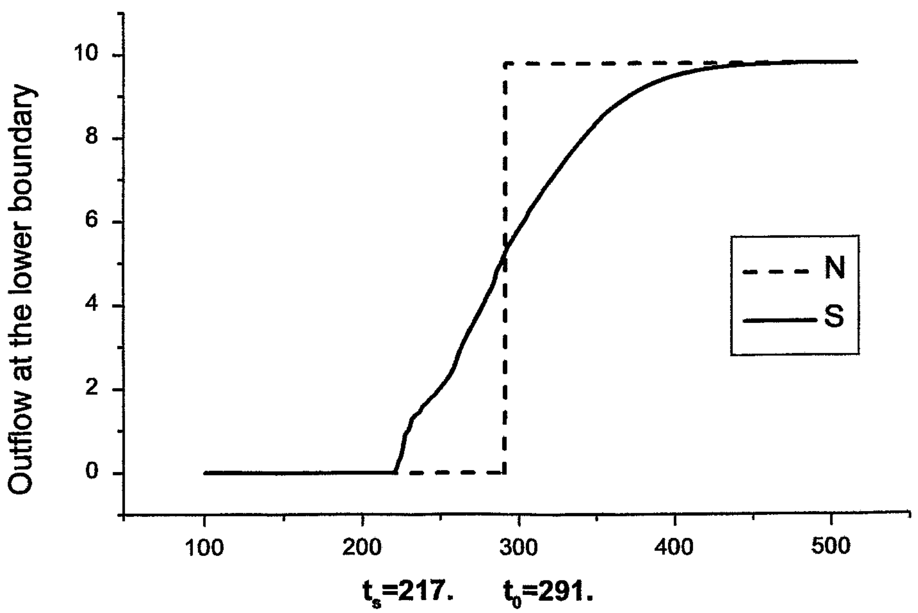


Fig. 9: Outflow of solute at the lower boundary for stochastic (S) and nonrandom (N) conductivity (Problem B, see details in text).

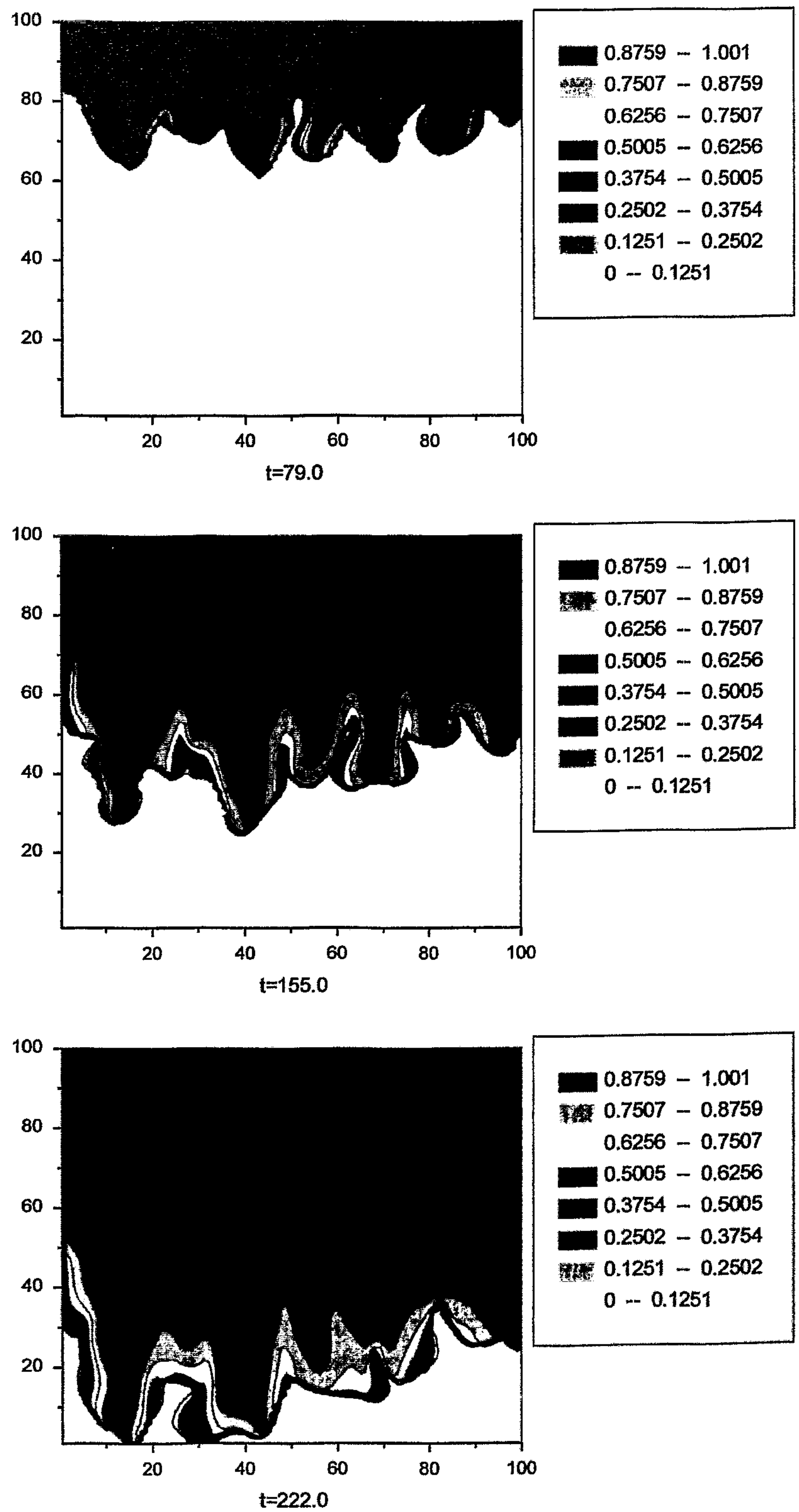


Fig. 8: Fields of solute concentration in a medium with stochastic conductivity at different times (numerical solution of Problem B; see details in text).

In the case of stochastic conductivity with mathematical expectation $\mathbf{E}K(x,y)=K_0$ the integral flux (8) may rather differ from the value determined by Eq. (9). Numerical experiments showed that the value F can be considerably smaller than F_0. In other words, an "effective" conductivity K_* of stochastic medium defined by equation

$$F_0 = (H_1 - H_0)K_* Y / X$$

is smaller than the conductivity K_0. Fig. 10 illustrates this effect in dependence on the variance S^2 of the random field of conductivity $K(x,y)$. These fields were sampled for correlation functions (4), (7) and parameters X=100, Y=100, K_0=1.

4. Conclusions and plans

The stochastic structure of the fields of hydraulic conductivity is a principal point that must be taken into account for investigations of solute transport in porous media. Some of the effects caused by random conductivity are rather different from those that can be described by introducing the dispersion term in the convection-dispersion equation (1) (see item C in section 3 and Fig. 11).

The presented first results suggest that the study of solute transport in stochastic porous media using up-to-date numerical models of random fields seems to be a promising direction of research. Therefore, the following items will be considered further on:

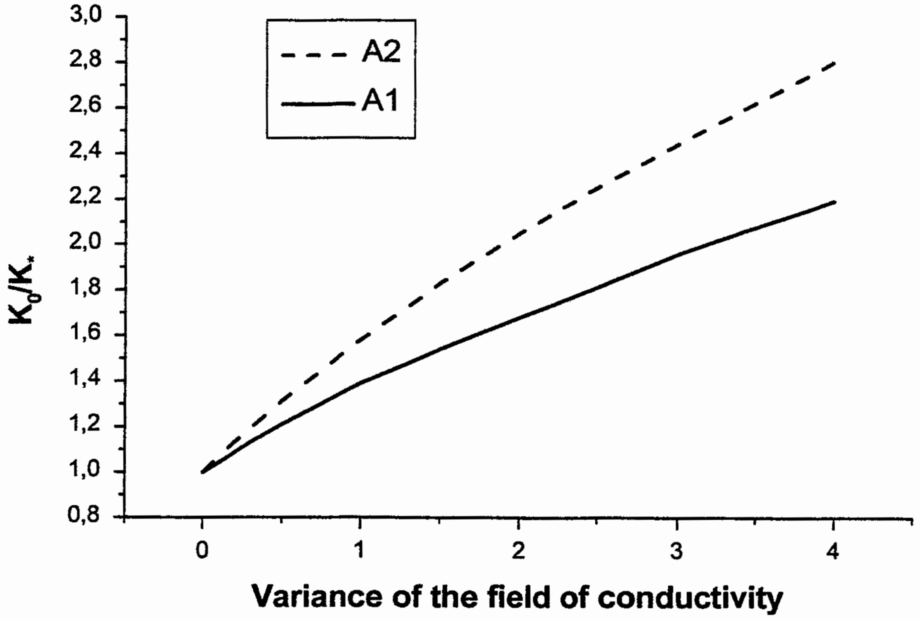
- to take into account the randomness of porosity as well as the randomness of conductivity;
- to elaborate the correspondent algorithms for solving problems in the three-dimensional case;
- to study the correlation between the stochastic convection term and the dispersion term of the convection-dispersion equation using theoretical methods and numerical experiments.

Appendix

Spectral models of random fields: basic principle and general algorithm

Let us consider a real homogeneous Gaussian random field $\xi(x)$, $\mathbf{x}\in\mathbf{R}^k$, with zero mean, unit variance and correlation function $R(\mathbf{x})=\mathbf{E}\xi(\mathbf{x}+\mathbf{y})\xi(\mathbf{y})$. The spectral representations of the random field and its correlation function are of the form (see, for example, [16]):

$$\xi(\mathbf{x}) = \int_P cos\langle \mathbf{x},\omega\rangle \varsigma(d\omega) + \int_P sin\langle \mathbf{x},\omega\rangle \eta(d\omega), \qquad (A1)$$



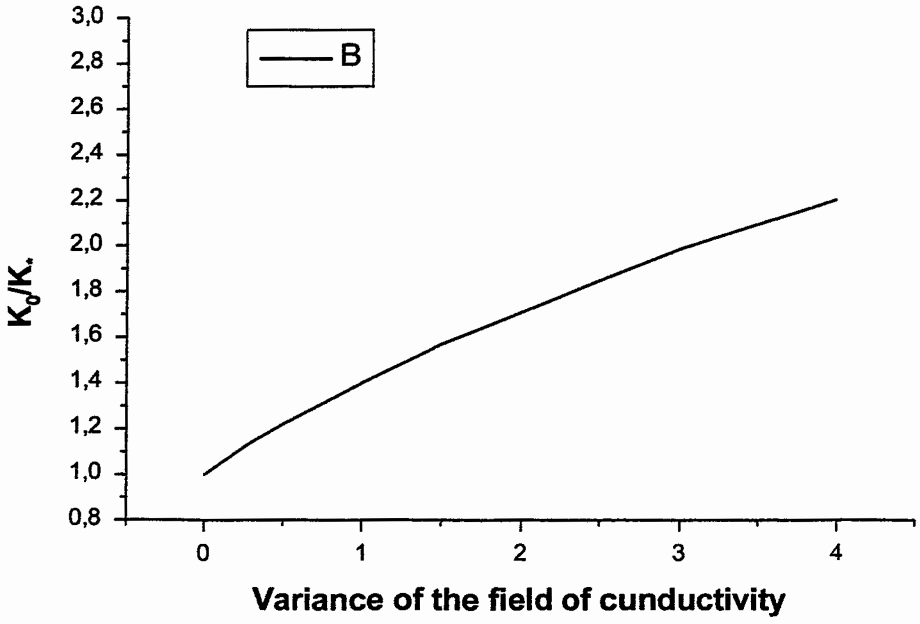


Fig. 10: The coefficient K_0/K_* of "effective conductivity decrease" in stochastic stochastic medium in dependence on the variance of the field of onductivity (see details in text): (A1) - model (3), (4), $\rho_x = 0.81$, $\rho_y = 0.81$; (A2) - model (3), (4), $\rho_x = 0.4$, $\rho_y = 0.81$; (B) - model (3), (7), $\lambda = 0.5$.

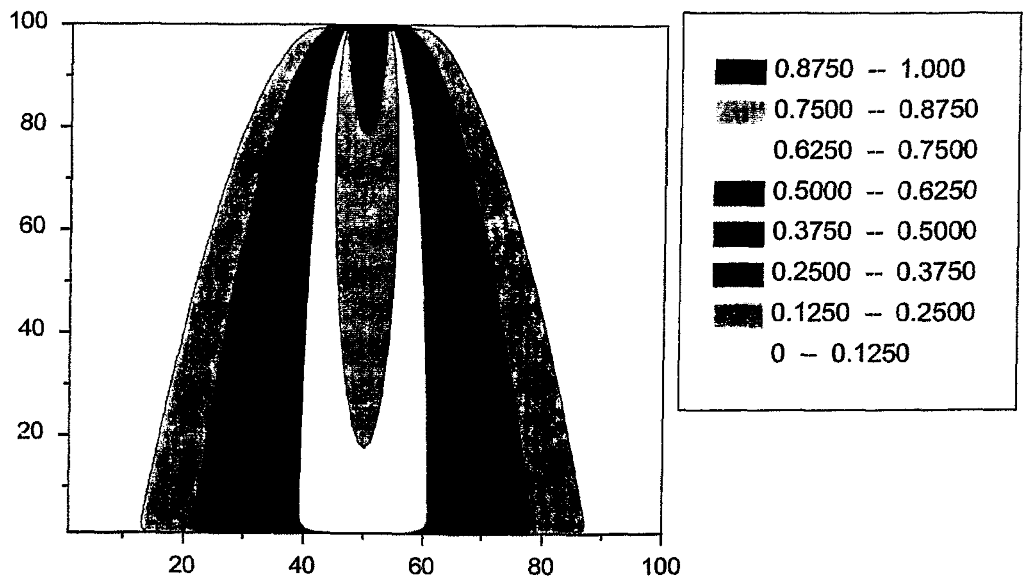


Fig. 11: Typical asymptotic distribution of solute concentration for Problems A and B with nonrandom conductivity and nonzero dispersion term.

$$R(\mathbf{x}) = \int_P \cos\langle \mathbf{x}, \omega \rangle m(d\omega).$$

Here $\zeta(d\omega)$, $\eta(d\omega)$ are real-valued orthogonal stochastic Gaussian measures on a half-space $\boldsymbol{P}$ that is called "spectral space" (i.e., $\boldsymbol{P}$ is a measurable set such that $\boldsymbol{P} \cap -\boldsymbol{P} = \{0\}$, $\boldsymbol{P} \cup -\boldsymbol{P} = \boldsymbol{R}^k$), $m(d\omega)$ is a spectral measure of the random field $\xi(\mathbf{x})$ and $\langle .,. \rangle$ denotes the scalar product in $\boldsymbol{R}^k$. In this case the following properties are fulfilled:

(1) $\mathbf{E}\zeta(A) = \mathbf{E}\eta(B) = 0,$

(2) $\mathbf{E}\zeta(A)\eta(B) = 0,$

(3) $\mathbf{E}\zeta^2(A) = \mathbf{E}\eta^2(A) = m(A),$

(4) If $A \cap B = \varnothing$, then $\mathbf{E}\zeta(A)\zeta(B) = \mathbf{E}\eta(A)\eta(B) = 0,$

where A and B stand for measurable subsets of $\boldsymbol{P}$.

The main idea underlying the methods of constructing the spectral models is to take an approximation of the stochastic integral (A1) as a numerical model of the random field $\xi(\mathbf{x})$. In general form a spectral model of homogeneous Gaussian random field $\xi(\mathbf{x})$ can be written as a sum of harmonics:

$$\xi_n(\mathbf{x}) = \sum_{j=1}^{n} a_j [\zeta_j \cos\langle \mathbf{x}, \omega_j \rangle + \eta_j \sin\langle \mathbf{x}, \omega_j \rangle]$$

where $a_j > 0$, ζ_j and η_j are independent random variables (usually Gaussian),

$$\mathbf{E}\zeta_j = \mathbf{E}\eta_j = \mathbf{E}\zeta_j\eta_k = 0, \qquad \mathbf{E}\zeta_j^2 = \mathbf{E}\eta_k^2 = 1,$$

and ω_j are random vectors distributed in spectral space $\boldsymbol{P}$. One of the most promising spectral models - the method of "spectrum splitting and randomisation" - was proposed first in [17].

Spectral models turned out to be a very effective tool for numerical modelling of various classes of Gaussian homogeneous random fields: scalar, vector-valued, isotropic, spatial-temporal, and etc. Some modifications of spectral models are used even for the simulation of non-Gaussian and non-homogeneous random fields. Detailed information on spectral models can be found in [11-13,18]. The simulations of isotropic Gaussian random fields of hydraulic conductivity on a plane area were performed according to the following formulas (for details see [12,13,18])

$$K(x,y) = exp(\sigma\xi_{NM}(x,y) + \mu),$$

$$\xi_{NM}(x,y) = (NM)^{-1/2}\sum_{j=1}^{N}\sum_{k=1}^{M}\sqrt{-2\ln\alpha_{jk}} \times cos[\rho_j(x\cos\chi_{jk} + y\sin\chi_{jk}) + 2\pi\beta_{jk}],$$

where $N{\times}M$ is the number of harmonics,

$$\chi_{jk} = \frac{\pi(k-\gamma_j)}{M},$$

α_{jk}, β_{jk}, γ_j are independent random variables uniformly distributed in [0,1], and ρ_j are independent random variables distributed in $[0,+\infty)$ according to the radial spectral density $g(\rho)$ of the Gaussian field

$$B(r) = \int_0^\infty J_0(r\rho)g(\rho)d\rho = \mathbf{E}\ \xi(x,y)\ \xi(0,0), \qquad r=(x^2+y^2)^{1/2}.$$

For $B(r)=\dfrac{sin(\lambda r)}{\lambda r}$ the radial spectral density g is given by

$$g(\rho) = \frac{\rho}{\lambda\sqrt{\lambda^2-\rho^2}}, \qquad \rho<\lambda,$$

for $B(r)=exp(-\lambda r)$

$$g(\rho) = \lambda\rho(\rho^2+\lambda^2)^{-3/2},$$

and for $B(r)=J_0(\lambda r)$ it is the delta-function $\delta(\lambda\text{-}\rho)$.

Acknowledgements

The first author wants to express his gratitude to Deutscher Akademischer Austauschdient for the support of this study. Also, he wants to thank Prof. F.-P. Weiß for giving the possibility to perform this research work in the Institut für Sicherheitsforschung of the Forschungszentrum Rossendorf.

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