

Geostatistical and stochastic concepts in groundwater

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Considerable problems in the formulation and application of subsurface water models are present in the treatment of the uncertainty of the parameter values (e.g., hydraulic conductivity), the initial and boundary conditions, or even in the formulation of the relevant processes themselves. The uncertainty of the parameters may be on the one hand due to measurement errors inherent in a specific evaluation method. On the other hand it is due to the strong spatial variability of many parameters (e.g., hydraulic conductivity), which never can be known in detail everywhere. Ways out of the dilemma are, e.g., to introduce stochastic concepts considering the aquifer as one of many possible stochastic realizations. Stochastic variables like the hydraulic conductivity do not behave like a white noise but show a distinct spatial correlation structure with the correlation between two values depending on their distance. This correlation structure may be characterized by, e.g., an auto-covariance function, or a variogram. A further important feature is the probability density function of the parameter under consideration. The hydraulic conductivity often is log-normally distributed, i.e., the log-transformed values fit a normal distribution.

A common approach in the practical application of models is to formulate effective or equivalent parameters thus replacing the real system by a homogeneous equivalent model. A series of analytical approximate expressions have been developed to estimate effective flow and pollutant transport parameters based on the knowledge of geostatistical parameters (probability density function, variance, correlation lengths, etc.). One example is the expression of the effective hydraulic conductivity given the covariance function. It can be shown, e.g., that in two-dimensions it simply becomes the geometric mean value provided that values are log-normally distributed and the correlation length is very small compared to the domain length. Another example is the approximate expression of the effective longitudinal and transversal dispersivities (or also called macrodispersivities), which are not constant but depend on the travel distance of the solute cloud and only asymptotically approach a constant value. These effective dispersivities characterize the spatial distribution of the solute cloud around the center of mass. The effect that the effective dispersivities generally increase for increasing travel distance is also observed in many field tracer tests. Approximate analytical models are also given for the consideration of a spatial variability of sorption and decay parameters of a dissolved substance.

Alternative procedures are, e.g., the use of Monte Carlo techniques by generating space-dependent (or also time-dependent) parameter values of numerical models in a stochastic manner, and the subsequent solution of each of the corresponding deterministic numerical systems. As example consider a flow domain. For this domain the hydraulic conductivity field is stochastically generated fulfilling a log-normal probability density function as well as a auto-covariance function and a mean value. It is possible to consider measured data in the stochastic generation process. With the help of a numerical groundwater model the corresponding flow field is calculated, which can be used to compute transport processes. For each realization one gets a corresponding result (hydraulic head.). The ensemble of results can be statistically analyzed thus reflecting the uncertainty in the expected result. However, Monte Carlo

techniques are often time consuming. Moreover it not always clear which number of realizations is necessary for the convergence of the method. Nevertheless they represent rather general and versatile tools for the investigation of spatially variable and/or uncertain parameters. An important application is the estimation of the uncertainty bandwidth of the result. Also the use of a stochastic generation of sedimentary units or facies elements with specific hydraulic properties is increasingly used.

1.1 Concepts and parameters

Most existing stochastic methods and models for flow and transport in groundwater (e. g., Journel und Huijbregts, 1978; Gelhar und Axness, 1983; Neuman et al., 1987; Dagan, 1989; Gelhar, 1993; Kitanidis, 1997; Zhang, 2002) start from ‘point’ values of hydraulic parameters, like hydraulic conductivity \mathbf{K} , transmissivity \mathbf{T} , porosity n , specific discharge \mathbf{v} , or piezometric head h . A ‘point’ value in groundwater is a **macroscopic entity** and is, e. g., related to averaging over a representative elementary volume REV (Bear, 1979), or a volume based on geostatistical criteria (Dagan, 1989). It’s required that the average over the volume is (practically) independent of the size of the volume. If D is the scale of the averaging volume, d the pore scale, and L the scale of the flow and transport domain, it’s required for a macroscopic quantity that $d \ll D \ll L$. According to a geostatistical point of view a macroscopic *quantity itself is subject to spatial variability. It is a random variable or space function $Z(\mathbf{x})$* . Figure 1 shows an example of a horizontal transect of hydraulic conductivity K taken in a visually homogeneous gravel layer (sedimentary type called grey gravel) (Jussel et al., 1994).

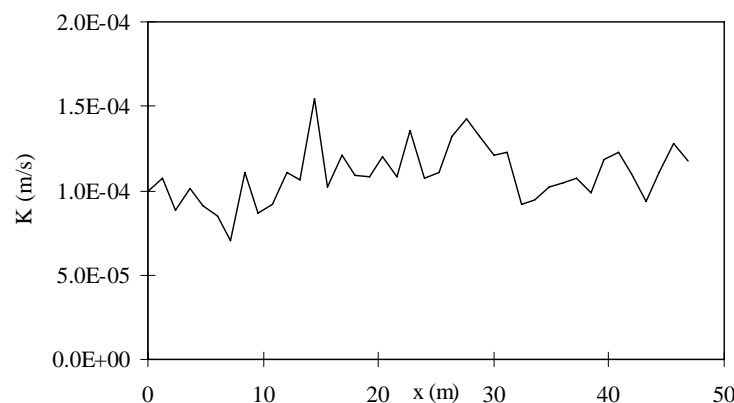


Fig. 1 Example of spatial variability: Horizontal transect of hydraulic conductivity K taken in a visually homogeneous gravel layer (called grey gravel), estimated from grain size analysis. (Jussel et al., 1994).

A basic property of random variables is the **probability density function** $f(Z)$. A frequent distribution is the well known **Gaussian or normal distribution**:

$$f(Z) = \frac{1}{\sqrt{2\pi}\sigma_Z} \cdot \exp\left(-\frac{[Z - \mu_Z]^2}{2\sigma_Z^2}\right)$$

with mean μ_Z and variance σ_Z^2 . Of special importance is the log-normal distribution $f(\ln(Z))$. Both are continuous distributions. Porosity $n(\mathbf{x})$ and piezometric head $h(\mathbf{x})$ are often considered as normally distributed. The absolute values or components of specific discharge $\mathbf{q}(\mathbf{x})$,

the hydraulic conductivity $\mathbf{K}(\mathbf{x})$ and the transmissivity $\mathbf{T}(\mathbf{x})$ values are often assumed as **log-normally distributed**. This is mainly due to the fact that the values are positive and relatively many small values exist compared to larger values.

In the context of random fields the statistical property of **ergodicity** is of importance. Applied to a groundwater system ergodicity tells us whether the single realization of an aquifer exhibits the same probability density function $f(Z(\mathbf{x}))$ as the ensemble.

Based on the probability density function **statistical moments** of various order can be defined. The first statistical moment of the random variable Z is the **mean** μ_Z :

$$\mu_Z = E[Z] = \int_{-\infty}^{\infty} Z f(Z) dZ$$

$E[Z]$ is the **expectation** of $Z(\mathbf{x})$. The second statistic moment of Z is the **variance** σ_Z^2 :

$$\sigma_Z^2 = \int_{-\infty}^{\infty} (Z - \mu_Z)^2 f(Z) dZ$$

The **variance** is a **measure for variability**. For hydraulic conductivity, assumed as log-normally distributed, the variance σ_Y^2 , with $Y = \ln(K)$ (natural logarithm) is dimensionless. In aquifers values for σ_Y^2 of 0.1 can be considered as small, whereas a value of 1 is large.

In the practical application of both the normal and the log-normal distribution it can be useful to **express mean and variance given the values of the corresponding log-normal distributions**. A log-normal random variable $X = \ln(Z)$ is normally distributed with mean μ_X . The mean of Z is (Gelhar, 1993):

$$\mu_Z = E[Z] = \int_{-\infty}^{\infty} Z f(Z) dZ = \exp\left(\mu_X + \frac{\sigma_X^2}{2}\right)$$

and the variance:

$$\sigma_Z^2 = E[(Z - \mu_Z)^2] = \int_{-\infty}^{\infty} (Z - \mu_Z)^2 f(Z) dZ = \exp(2\mu_X + \sigma_X^2) \cdot [\exp(\sigma_X^2) - 1]$$

From a stochastic point of view a spatially variable entity $Z(\mathbf{x})$ or $Z(\mathbf{x}, t)$ with $\mathbf{x} = (x, y, z)$ can be interpreted as one single realization of a **random variable** $Z(\mathbf{x})$ or $Z(\mathbf{x}, t)$. All possible realizations together are called the **ensemble**. At a particular location \mathbf{x} the expected value for the **mean** over all possible realizations is:

$$\mu_Z(\mathbf{x}) = E[Z(\mathbf{x})]$$

and the **covariance** for any pair of two locations \mathbf{x} and \mathbf{x}' (two-point covariance) is:

$$R_Z(\mathbf{x}, \mathbf{x}') = E[(Z(\mathbf{x}) - \mu_Z(\mathbf{x})) \cdot (Z(\mathbf{x}') - \mu_Z(\mathbf{x}'))]$$

For $\mathbf{x} = \mathbf{x}'$ the covariance $R_Z(\mathbf{x}, \mathbf{x})$ yields the variance $\sigma_Z^2(\mathbf{x})$. Correspondingly, the **cross-covariance** for any pair of random variables at two locations $X(\mathbf{x})$ and $Z(\mathbf{x}')$ is:

$$R_{ZZ}(\mathbf{x}, \mathbf{x}') = E[(Z(\mathbf{x}) - \mu_Z(\mathbf{x})) \cdot (Z(\mathbf{x}') - \mu_Z(\mathbf{x}'))]$$

In stochastic theories it is often assumed that random variables are **stochastically stationary** or homogeneous. A stochastically stationary spatial random variable does not show spatial trends in mean and average, and in the higher statistical moments (Fig. 2). Generally speaking the expectation for statistical moments in the neighbourhood for an arbitrary location \mathbf{x} is independent of space. Stationarity up to the second order does therefore imply that mean μ_Z and variance σ_Z^2 as well as the covariance are independent of \mathbf{x} and therefore invariant.

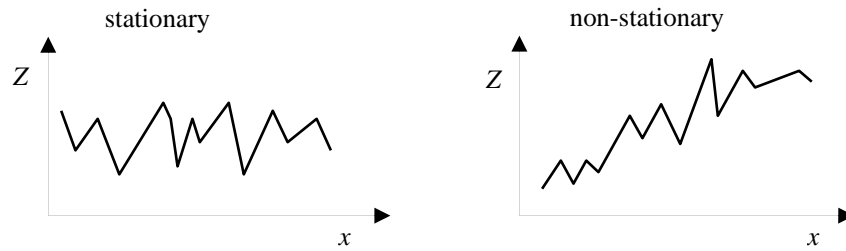


Fig. 2 Stationary and non-stationary random space variable $Z(\mathbf{x})$ (schematically).

1.1.1 Covariance function

For a stationary random variable the mean $\mu_Z(\mathbf{x})$ is constant:

$$\mu_Z = E[Z(\mathbf{x})]$$

and the two-point covariance $R_Z(\mathbf{x}, \mathbf{x}')$ depends only on the separation vector $\mathbf{s} = \mathbf{x} - \mathbf{x}'$ between two locations \mathbf{x} and \mathbf{x}' and is therefore invariant:

$$R_Z(\mathbf{x}, \mathbf{x}') = R_Z(\mathbf{s}) = E[(Z(\mathbf{x}) - \mu_Z) \cdot (Z(\mathbf{x} + \mathbf{s}) - \mu_Z)]$$

It is often called **covariance function** or auto-covariance function (Fig. 3). For $\mathbf{s} = 0$ the covariance function $R_Z(\mathbf{s} = 0) = \sigma_Z^2$ reduces to the variance of $Z(\mathbf{x})$. Often, for $s \rightarrow \infty$ the covariance function approaches zero. For expressing the covariance function it is necessary that the mean μ_Z is known.

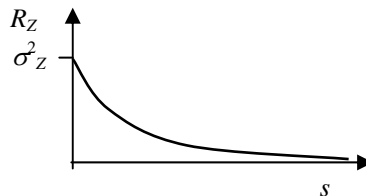


Fig. 3 Covariance function $R_Z(\mathbf{s})$ (schematically).

The covariance function $R_Z(\mathbf{s})$ enables an assessment of the spatial correlation of $Z(\mathbf{x})$. The covariance function is related to the **correlation function** or auto-correlation function $\rho_Z(\mathbf{s})$ by:

$$R_Z(\mathbf{s}) = \sigma_Z^2 \rho_Z(\mathbf{s})$$

with $\rho_Z(\mathbf{s}=0)=1$. Several **covariance models** exist. A frequently used model is the **exponential covariance model**:

$$R_Z(\mathbf{s}) = \sigma_Z^2 \exp\left[-\frac{s}{I_Z}\right]$$

The parameter I_Z is the **correlation length**. In this formulation the model is isotropic since it does not depend on the orientation of the vector \mathbf{s} . However, the covariance function can be anisotropic. Accordingly, the corresponding random variable $Z(\mathbf{x})$ therefore is stochastically anisotropic. The **anisotropic exponential covariance model** is:

$$R_Z(\mathbf{s}) = \sigma_Z^2 \exp\left[-\sqrt{\left(s_x/I_x\right)^2 + \left(s_y/I_y\right)^2 + \left(s_z/I_z\right)^2}\right]$$

The parameters I_x , I_y , and I_z are the correlation lengths in the directions x , y , and z .

The correlation length indicates over which distance two values of $Z(\mathbf{x})$ are still correlated. In the special case of $I=0$ an uncorrelated random variable is obtained. In general, the **correlation length** (integral scale) is defined as:

$$I_i = \int_0^{\infty} \rho_Z(s_i) ds_i; \quad i = x, y, z$$

provided the integral yields a finite value.

The **cross covariance function** $R_{XZ}(\mathbf{s})$ is defined for two stationary random variables $X(\mathbf{x})$ and $Z(\mathbf{x})$ as:

$$R_{XZ}(\mathbf{s}) = E\left[\left(X(\mathbf{x}) - \mu_X\right) \cdot \left(Z(\mathbf{x} + \mathbf{s}) - \mu_Z\right)\right]$$

One example is the cross covariance function $R_{Yh}(\mathbf{s})$ with $Y(\mathbf{x}) = \ln(K(\mathbf{x}))$ and the piezometric head $h(\mathbf{x})$ indicating the correlation between these two variables.

Analytical approximate expressions for covariance and cross covariance functions of various variables for uniform mean flow can be found, e. g., in Dagan (1989) or Gelhar (1993).

1.1.2 Variogram

If the mean μ_Z of a random function $Z(x)$ is not a priori known, it is convenient use the **variogram** γ_Z (Fig. 4). It is defined as (Journel und Huijbregts, 1978):

$$\gamma(\mathbf{s}) = \frac{1}{2} E\left[\left(Z(\mathbf{x} + \mathbf{s}) - Z(\mathbf{x})\right)^2\right] = \frac{1}{2} \text{var}\left[\left(Z(\mathbf{x} + \mathbf{s}) - Z(\mathbf{x})\right)^2\right]$$

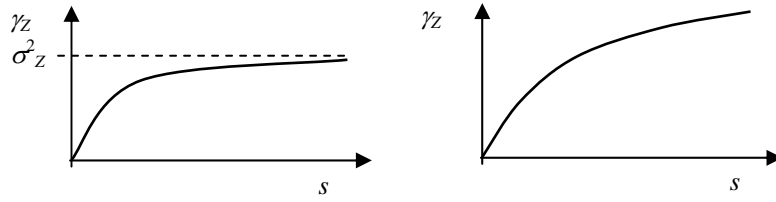


Fig. 4 Variogram $\gamma_Z(s)$ of a random variable $Z(\mathbf{x})$ (schematically); with finite (left) and with infinite variance (right)

The variogram represents half of the mean quadratic increment $Z(\mathbf{x}+\mathbf{s}) - Z(\mathbf{x})$ for two arbitrary points \mathbf{x} and $\mathbf{x}+\mathbf{s}$ with the lag \mathbf{s} . It can be interpreted as variance of the increment. The increment needs to be stationary. Compared to the covariance function the variogram is therefore more general and sometimes called weakly stationary. For stationary increments up to second order the mean and variance of the increment are:

$$\begin{aligned} E[Z(\mathbf{x}+\mathbf{s}) - Z(\mathbf{x})] &= \mu(\mathbf{s}) \\ E[(Z(\mathbf{x}+\mathbf{s}) - Z(\mathbf{x}))^2] &= f(\mathbf{s}) \end{aligned}$$

Usually it is assumed that $E[Z(\mathbf{x}+\mathbf{s}) - Z(\mathbf{x})] = 0$. A property of the variogram is that $\gamma(-\mathbf{s}) = \gamma(\mathbf{s})$. Theoretically, the variogram is for zero lag equal to $\gamma(s=0) = 0$. However, experimental variograms sometimes exhibit a non-zero value (Fig. 5), which is called ‘**nugget effect**’ (Journel and Huijbregts, 1978) and interpreted as impact of small-scale variability. In practice a value for $\gamma(s=0) > 0$ is often the result of an uncorrelated portion of $Z(\mathbf{x})$, e. g., measurement errors. If a random variable $Z(\mathbf{x})$ includes an **uncorrelated random variable** $\Delta(x,y,z)$ the variogram for $Z(\mathbf{x})$ reads:

$$\begin{aligned} \gamma_Z(\mathbf{s}) &= \frac{1}{2} E[(Z(\mathbf{x}+\mathbf{s}) - Z(\mathbf{x}))^2] = \frac{1}{2} E[(Z'_i + \Delta_i - Z'_j + \Delta_j)^2] \\ &= \frac{1}{2} E[(Z'_i - Z'_j)^2] + \frac{1}{2} E[\Delta_i^2 + \Delta_j^2] = \frac{1}{2} E[(Z'_i - Z'_j)^2] + \sigma_u^2 \\ &= \gamma(\mathbf{s}) + \sigma_u^2 \end{aligned}$$

σ_u^2 is the variance of the uncorrelated portion of Z . Such a variance is therefore additive to the correlated variogram $\gamma(\mathbf{s})$.

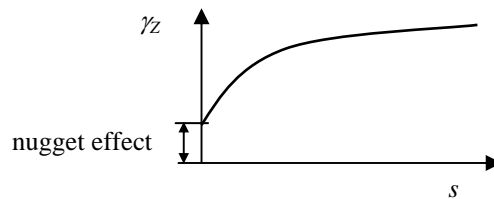


Fig. 5 Variogram with nugget effect

For a **stationary random variable** $Z(\mathbf{x})$, characterized by the covariance function $R_Z(\mathbf{s})$, (Fig. 6):

$$R_Z(\mathbf{s}) = E[\{Z(\mathbf{x}) - \mu_Z\} \cdot \{Z(\mathbf{x} + \mathbf{s}) - \mu_Z\}] = E[Z(\mathbf{x}) \cdot Z(\mathbf{x} + \mathbf{s})] - \mu_Z^2 []$$

the corresponding variogram is:

$$\begin{aligned} \gamma(\mathbf{s}) &= \frac{1}{2} \cdot E[(Z(\mathbf{x} + \mathbf{s}) - Z(\mathbf{x}))^2] \\ &= \frac{1}{2} \cdot E[\{Z(\mathbf{x} + \mathbf{s})\}^2] - E[Z(\mathbf{x} + \mathbf{s}) \cdot Z(\mathbf{x} + \mathbf{s})] + \frac{1}{2} E[\{Z(\mathbf{x})\}^2] \\ &= \frac{1}{2} \cdot (\sigma_Z^2 + \mu_Z^2) - (R_Z(\mathbf{s}) + \mu_Z^2) + \frac{1}{2} \cdot (\sigma_Z^2 + \mu_Z^2) \\ &= \sigma_Z^2 - R_Z(\mathbf{s}) \end{aligned}$$

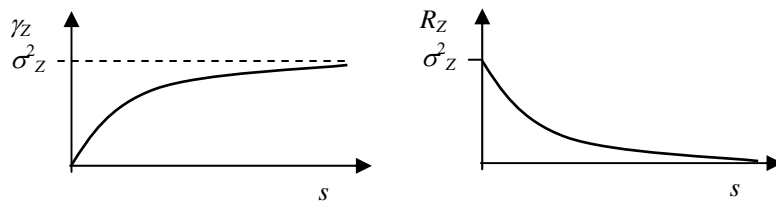


Fig. 6 Variogram $\gamma_Z(s)$ (left) for given covariance function $R_Z(s)$ (right)

Therefore, for stationary random variables the variogram is complementary to the covariance function. The asymptotic value is finite and equals the variance.

Various **theoretical variogram models** exist (de Marsily, 1983). Often used models are the **exponential variogram model**, here the isotropic version with the parameters variance σ_Z^2 and correlation length I_Z :

$$\gamma_Z(\mathbf{s}) = \sigma_Z^2 \cdot \left[1 - \exp\left(-\frac{|\mathbf{s}|}{I_Z}\right) \right]$$

or the **function with exponent p** :

$$\gamma_Z(\mathbf{s}) = a \cdot |\mathbf{s}|^p; \quad p, a \text{ constant}$$

With $p=1$ a linear variogram is obtained. Anisotropic models are formulated similar to covariance models.

What would be the **variogram of a linear deterministic function** $Z=Z_0+a x$ without random variable, and with constant Z_0 and a . The variogram yields $\gamma_Z(s)=a^2s^2$. Consequently we can assume that a quadratic variogram can be the result of a linear trend of a random variable $Z(\mathbf{x})$. Assuming a linear trend in the random variable $Z(x)$ with:

$$Z(\mathbf{x}) = Z_0 + Z'(\mathbf{x}) + \mathbf{I} \cdot \mathbf{x} = Z_0 + Z'(\mathbf{x}) + I_x x + I_y y + I_z z$$

with constant Z_0 and regression vector \mathbf{I} and a random residuum $Z'(\mathbf{x})$ the variogram is formulated for the residuum only (Dagan, 1989):

$$\gamma_z(\mathbf{s}) = \frac{1}{2} E[(Z'(\mathbf{x} + \mathbf{s}) - Z'(\mathbf{x}))^2]$$

In this context it should be mentioned that all parameters in groundwater may exhibit **trends** in their statistical moments. Moreover, certain variables like piezometric head $h(\mathbf{x})$ must have a trend of the mean value if groundwater flow is present. Additional problems arise when space dependent parameters are also **time dependent**, like the recharge rate $N(\mathbf{x}, t)$, the piezometric head $h(\mathbf{x}, t)$, or the specific discharge $\mathbf{q}(\mathbf{x}, t)$.

1.2 Analysing spatial variability of aquifer parameters

1.2.1 Practical determination of hydraulic parameters

Several field methods are available for the determination of hydraulic parameters like hydraulic conductivity K , porosity n , piezometric head h , storativity S (see, e. g., Hamill and Bell, 1986). In general every method is related to a **measurement scale**. Some of the most common methods are briefly characterized as follows:

1. **Measurement of the piezometric head h** in piezometers or wells. The values obtained depend on the perforation of the well casing. Therefore, the head measurement h is representative for the perforated section of the piezometer or well (complete perforated profile, or perforated section, or single opening). Therefore the measurement volume can be quite different. A further possibility consists of burying pressure cells in the aquifer in order to obtain 'point' values.
2. **Extraction of disturbed aquifer samples** in outcrops. From grain size analysis rough estimates of hydraulic conductivity K can be obtained. If the sample volume can be measured, the porosity n can be determined as well. The size of the sample should be based on consideration concerning a representative elementary volume. For such a sample 'point' values can be obtained.
3. **Extraction of undisturbed aquifer samples** in outcrops. By performing flow experiments the hydraulic conductivity K can be determined. Samples can also be analysed upon porosity n . The size of the sample should again be based on consideration concerning a representative elementary volume, yielding 'point' values.
4. Conducting **short range** (short time) **pumping tests** in wells or boreholes. The layout can include additional observation boreholes or piezometers. With such tests hydraulic conductivity K and transmissivity T can be estimated, and if possible, also storativity S . The results are valid only for the close surrounding of the perforated section of the well or borehole. If the aquifer is heterogeneous and consists of mainly horizontal layers in the surrounding of the well or borehole the hydraulic conductivity K corresponds to the arithmetic mean \overline{K} over the perforated section d :

$$\bar{K} = \int_{z=0}^d K(z) dz$$

5. Conducting **flowmeter measurements** in wells or boreholes. With such a device the hydraulic conductivity can be determined for a sequence of vertical layers Δz . Again the values obtained can often be interpreted as arithmetic mean over the section Δz :

$$\bar{K}_{\Delta z} = \int_{z=0}^{\Delta z} K(z) dz$$

An alternative is the dipole test in wells or boreholes (Zlotnik und Ledder, 1996) with withdrawal and injection sections. With such an arrangement values for K can be determined for sectors.

6. Conducting **large range** (large time) **pumping tests** in wells or boreholes with one or several piezometers for head observations. With such an experiment domain values of hydraulic conductivity K can be determined. Therefore, they are representative for a larger surrounding of the well or borehole.

With the exception of point 6 all methods are in principal suited for a geostatistical analysis. A problem often consists in the low **number of measurement locations** available. All determined or estimated values are always related to their **measurement scale** or volume of the particular method. Using methods 4 and 5 yield K -values representative over a specific section or thickness. This holds also for the estimated average K or variance σ^2_K , where K is approximately the arithmetic mean over the thickness H , a section d or layer Δz . Since we are sometimes interested in variance and correlation length of 'point'-values for $Y=\ln(K)$, we need further theoretical considerations (Stauffer, 1998).

In the following some **common tools for a geostatistical analysis** of field data are compiled. We presume that all data are related to a similar measurement scale or volume.

1.2.2 Estimation of variance

Given m uncorrelated values Z_i of a variable Z the estimated **variance** is:

$$\sigma_{Z,est}^2 = \text{Var}(Z) = \frac{1}{m-1} \sum_{i=1}^m (Z_i - \bar{Z})^2$$

Given m values, and assuming normal distribution the confidence limits for the variance can be assessed as:

$$a_l \sigma_{est}^2 \leq \sigma^2 \leq a_u \sigma_{est}^2$$

σ_{est}^2 is the estimation of the variance. The values a_l and a_u for a 95% confidence interval are listed in Table 1. Obviously, as well known, the uncertainty in the estimated variance for a small number of measurements is extremely large. The situation can be even worse for correlated data.

m	a_l	a_u
5	0.360	8.33
10	0.474	3.33
20	0.578	2.13
30	0.635	1.81
40	0.671	1.65
50	0.698	1.56
100	0.773	1.35

Table 1: Coefficients for 95% confidence interval of an estimated variance dependent on the number m of observations

1.2.3 Estimation of the one-dimensional covariance function

Given a series of Z_i values with constant distance Δz between neighbouring locations the estimation for the covariance function for lag distances of $s=k\Delta z$ is:

$$R_z(k \Delta z) = \frac{1}{m-k-1} \sum_{i=1}^{m-k} (Z_i - \bar{Z}) \cdot (Z_{i+k} - \bar{Z})$$

\bar{Z} is the estimation of the **arithmetic mean** of Z :

$$\bar{Z} = \frac{1}{m} \sum_{i=1}^m Z_i$$

1.2.4 Variogram estimation

The variogram is particularly suited for irregularly distributed measurement locations in a plane or in space. All possible pairs of points are considered. The variogram is estimated for given classes of lag distances s between the measurement locations. For distance class k with distances in the interval $[s_{k,\min}, s_{k,\max}]$ $m(k)$ pairs are registered, and the estimation of the variogram for the distance class k is:

$$\gamma_z(k) = \frac{1}{4m(k)} \sum_{i=1}^{m(k)} \sum_{j=1}^{m(k)} (Z_i - Z_j)^2$$

Z_i and Z_j are the measurements at locations i and j . The value $\gamma(k)$ is attributed to the average lag distance $\bar{s}(k)$ in class k :

$$\bar{s}(k) = \frac{1}{m(k)} \sum_{i=1}^{m(k)} s_i$$

An example of a variogram is given in Fig. 7. It is based on the measurements of $Y=\ln(K)$ shown in Fig. 1. The nugget effect is interpreted as uncorrelated measurement error. An exponential variogram model was fitted.

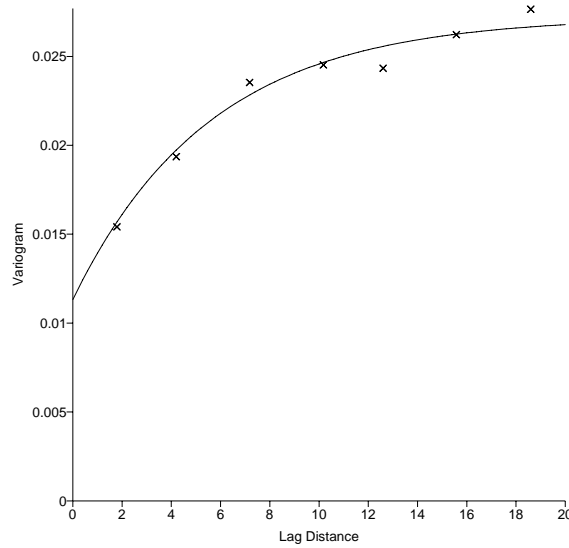


Fig. 7 Experimental and theoretical variogram of $Y=\ln(K)$ of the series of 40 K -values shown in Fig. 1. Exponential variogram model (solid line) with nugget effect $\sigma^2_Y=0.011$, variance $\sigma^2_Y=0.016$ and horizontal correlation length $\lambda_{Y,hor}=5.6m$.

The **accuracy of the variogram** estimation much depends on the number of measurement locations. Journel and Huijbregts (1978) suggest that the number of pairs in a distance class should not be less than about 30 to 50. For a small number of data only very rough estimates of the variance and the correlation length can be obtained. Moreover, the variogram should be analysed only to about half of the maximum distance of the domain, since for larger lag distances only restricted sampling is possible, which are not representative.

1.3 Interpolation and averaging using geostatistics: Kriging

A frequent practical problem is spatial **interpolation** or **averaging** given measurements of a variable at discrete locations (Delhomme, 1987; de Marsily; 1986, Kitanidis, 1997). A further salient question is the assessment of the accuracy of the interpolation or the average. Obviously spatial variability and correlation has to be taken into account. Given a series of measurements Z_i at discrete locations $\mathbf{x}_i(i=1,n)$ what is the **expected value** Z_0^* at an arbitrary location \mathbf{x}_0 , or what is the **expected average** within an arbitrary domain (area, volume), taking into account spatial variability? Furthermore, what is the **estimation variance**? The estimate may be written as a **weighted sum** over all measurements Z_i :

$$Z_0^* = \sum_{i=1}^n \lambda_{0,i} Z_i$$

The parameters $\lambda_{0,i}$ are the (yet unknown) kriging weights for the pair of points P_0-P_i . The symbol n is the number of measurements. All measurements contribute to the estimate depending on their weight. For an **unbiased estimate** the following condition has to be fulfilled:

$$E\left[\sum_{i=1}^n \lambda_0^i Z_i\right] = \sum_{i=1}^n \lambda_0^i E[Z_i] = \mu$$

In order to be unbiased Z_0^* is considered as single observation of a random variable and Z_i are quantities of n random variables with the expectation:

$$E[Z_i] = \mu$$

This leads to the condition for the weights:

$$\sum_{i=1}^n \lambda_0^i = 1$$

Imagine an infinite number of realizations of **random fields** $Z(\mathbf{x})$, honouring all the measurements and also fulfilling a given variogram. The ensemble of realizations contains all possible values and therefore the expectation and the variance at any arbitrary location \mathbf{x} . Therefore for the determination of the kriging weights it is required that the **estimation variance is minimum** (de Marsily, 1986):

$$E\left[\left(Z_0^* - Z_0\right)^2\right] = E\left[\left(\sum_{i=1}^n \left(\lambda_0^i Z_i\right) - Z_0\right)^2\right] = \sum_{i=1}^n \sum_{j=1}^n \lambda_0^i \lambda_0^j \cdot E\left[\left(Z_i - Z_0\right) \cdot \left(Z_j - Z_0\right)\right] \rightarrow \min.$$

The variable Z_0 is the (unknown) true value at location \mathbf{x}_0 . From the variogram follows:

$$\gamma(\mathbf{x}_i - \mathbf{x}_j) = \gamma(\mathbf{x}_i - \mathbf{x}_0) + \gamma(\mathbf{x}_j - \mathbf{x}_0) - E\left[\left(Z_i - Z_0\right) \cdot \left(Z_j - Z_0\right)\right]$$

Therefore the minimum variance is:

$$E\left[\left(Z_0^* - Z_0\right)^2\right] = -\sum_{i=1}^n \sum_{j=1}^n \lambda_0^i \lambda_0^j \gamma(\mathbf{x}_i - \mathbf{x}_j) + 2\sum_{i=1}^n \sum_{j=1}^n \lambda_0^i \lambda_0^j \gamma(\mathbf{x}_i - \mathbf{x}_0)$$

This leads to the problem of finding the **minimum with constraints**:

$$\frac{1}{2} E\left[\left(Z_0^* - Z_0\right)^2\right] - \varepsilon \cdot \left[\sum_{i=1}^n \lambda_0^i - 1\right] \rightarrow \min.$$

The parameter ε is the Lagrange multiplier, yet unknown. The resulting equation system for the kriging weights is linear:

$$\begin{aligned} \sum_{i=1}^n \lambda_0^i \gamma(\mathbf{x}_i - \mathbf{x}_j) + \varepsilon &= \gamma(\mathbf{x}_i - \mathbf{x}_0); & i = 1, 2, \dots, n \\ \sum_{i=1}^n \lambda_0^i &= 1 \end{aligned} \tag{1}$$

or in matrix and vector notation:

$$\begin{bmatrix} 0 & \gamma_{12} & \dots & \gamma_{1n} & 1 \\ \gamma_{21} & 0 & \dots & \gamma_{2n} & 1 \\ \dots & \dots & 0 & \dots & 1 \\ \gamma_{n1} & \gamma_{n2} & \dots & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix} \cdot \begin{Bmatrix} \lambda_0^1 \\ \lambda_0^2 \\ \dots \\ \lambda_0^n \\ \varepsilon \end{Bmatrix} = \begin{Bmatrix} \gamma_{10} \\ \gamma_{20} \\ \dots \\ \gamma_{n0} \\ 1 \end{Bmatrix}$$

with $\gamma_{ij}=\gamma(\mathbf{x}_i-\mathbf{x}_j)$. As soon as the kriging weights λ_0^i are determined the estimate Z_0^* at location \mathbf{x}_0 can be calculated. It has to be noted that only a **limited class of variogram models** can be accepted (de Marsily 1986). In order to obtain a unique solution of the linear equation system it is required that the increase in the variogram function $\gamma(s)$ for increasing s is smaller than s^2 , e. g., in the function with exponent a :

$$\gamma(s) = \omega |s|^a; \quad a < 2$$

The equation system 1 contains only information on the measurement locations but no measured data. Furthermore information on point P_0 is only present in the constant vector. Therefore the kriging matrix has to be inverted only once. The kriging weights can be obtained for any arbitrary location \mathbf{x}_0 using the inverted matrix. As soon as the kriging weights are known, the **estimation variance** can be determined. Starting from Eq. 1 the estimation variance is:

$$\text{Var}(Z_0^* - Z_0) = \sigma^2 = \sum_{i=1}^n \lambda_0^i \gamma(\mathbf{x}_i - \mathbf{x}_0) + \varepsilon$$

Again no measured data is used. Therefore kriging enables not only an estimate but also an estimate of the variance. Both estimate and variance form a couple. The true value is expected within a bandwidth given by the estimate Z_0^* and the variance. Assuming Gaussian distribution of Z_0^* leads to a determination of Gaussian confidence intervals. The estimate at a measurement location \mathbf{x}_i leads to variance zero. Therefore, kriging using Eq. 1 is an exact interpolator.

It is further possible to obtain an **estimate of the arithmetic average over a domain**, e. g. an area. This can be an arbitrary domain or a finite element, or a finite difference cell. The average of a random variable $Z(\mathbf{x})$ over the area A_0 is:

$$\bar{Z}_0 = \frac{1}{A_0} \int_{A_0} Z(\mathbf{x}) dA$$

and is again a weighted average over all measurements:

$$\bar{Z}_0^* = \sum_{i=1}^n \lambda_0^i Z_i$$

The requirement of minimum estimation variance and of unbiased estimate leads to the following equation system:

$$\sum_{i=1}^n \lambda_0^i \gamma(\mathbf{x}_i - \mathbf{x}_j) + \varepsilon = \bar{\gamma}(\mathbf{x}_i - \mathbf{x}_j); \quad i = 1, 2, \dots, n$$

$$\sum_{i=1}^n \lambda_0^i = 1$$

The system contains the averaged variogram:

$$\bar{\gamma}(\mathbf{x}_i - \mathbf{x}_0) = \frac{1}{A_0} \int_{A_0} \gamma(\mathbf{x}_i - \mathbf{x}_0) dA$$

The estimation variance of the variable is:

$$\text{Var}(Z_0^* - Z_0) = \sigma^2 = \sum_{i=1}^n \lambda_0^i \bar{\gamma}(\mathbf{x}_i - \mathbf{x}_0) + \varepsilon - \bar{\bar{\gamma}}$$

with $\bar{\bar{\gamma}} = \frac{1}{A_0^2} \int_{A_0} \int_{A_0} \gamma(\mathbf{x} - \mathbf{y}) dA_x dA_y$

Generally, by means of an averaging procedure the estimation variance is reduced.

A further generalization of kriging can be obtained by **considering a variance of the measurements** σ_i^2 different from zero of the measurements Z_i , assuming:

- Measurement errors are not systematic.
- Measurements are uncorrelated among each other.
- Measurements are uncorrelated with the random field Z.
- The variance is a priori known.

The estimate at location \mathbf{x}_0 is again a weighted average of the measurement. The resulting equation system is:

$$\sum_{i=1}^n \lambda_0^i \gamma(\mathbf{x}_i - \mathbf{x}_j) - \lambda_0^i \sigma_i^2 + \varepsilon = \gamma(\mathbf{x}_i - \mathbf{x}_0); \quad i = 1, 2, \dots, n$$

$$\sum_{i=1}^n \lambda_0^i = 1$$

or:

$$\begin{bmatrix} \sigma_1^2 & \gamma_{12} & \dots & \gamma_{1n} & 1 \\ \gamma_{21} & \sigma_2^2 & \dots & \gamma_{2n} & 1 \\ \dots & \dots & \dots & \dots & 1 \\ \gamma_{n1} & \gamma_{n2} & \dots & \sigma_n^2 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \lambda_0^1 \\ \lambda_0^2 \\ \dots \\ \lambda_0^n \\ \varepsilon \end{bmatrix} = \begin{bmatrix} \gamma_{10} \\ \gamma_{20} \\ \dots \\ \gamma_{n0} \\ 1 \end{bmatrix}$$

and the estimation variance:

$$\text{Var}(Z_0^* - Z_0) = \sigma^2 = \sum_{i=1}^n \lambda_0^i \gamma(\mathbf{x}_i - \mathbf{x}_0) + \varepsilon$$

The estimate at measurement locations now does not necessarily meet the measurements exactly any more.

The kriging procedure as shown needs the variogram of Z . The mean of Z remains unknown. This is referred to as **kriging in the intrinsic case**. Kriging can also be performed for given covariance function of Z and given the mean of Z . This results in a kriging system without Lagrange operator. The procedure is referred to as **kriging in the stationary case** (de Marsily, 1986).

Stochastic stationarity may be a question of scale. A random function may be, e. g.,:

- Stationary over a large distance.
- Non-stationary over medium distances.
- Stationary over short distances.

Non-stationary behaviour can be considered, e.g., by following techniques:

- **Remove trend function**. This needs to be uncorrelated with the data.
- **Universal kriging** (Journel und Huijbregts, 1978).
- **Kriging with Intrinsic Random Function of Order k** (de Marsily, 1986, Kitanidis, 1997).

The result of kriging for a specific application can easily be **verified** by omitting one measurement at location \mathbf{x}_i and by calculating estimate and variance at that location. The measurement is supposed to be within the estimated confidence interval. An interesting application of kriging lies in the assessment and **optimisation of a monitoring network**.

A special case is **indicator kriging** (Journel und Huijbregts, 1978). The random variable $Ind(\mathbf{x})$ is binary with $Ind=1$ (The considered property is met at location \mathbf{x}) and $Ind=0$ (The property is not met at location \mathbf{x}). In the kriging system $Z(\mathbf{x})$ is replaced by $Ind(\mathbf{x})$ and the variogram by the indicator variogram. The estimate $Z^*(\mathbf{x})$ is now the probability $p(\mathbf{x})$ of the property P being $Ind=1$ at location \mathbf{x} .

1.4 Numerical stochastic simulation, Monte Carlo techniques

Numerical stochastic simulation is performed by the **generation of a random field** of a random variable $Z(\mathbf{x})$ at discrete locations using a random generator. This random generator has to meet the probability density function, the variance, and the spatial correlation structure. For example a field of hydraulic conductivity $K(\mathbf{x})$ can be generated fulfilling a log-normal distribution and a given mean and covariance function. No further restrictions as small variance are required. The generation process may be conditioned by **honouring measured data** Z_i thus leading to a **conditional stochastic simulation**. In case of no conditions we get an **unconditional stochastic simulation**. The number of random variables may be arbitrary. For example we may stochastically generate a field of hydraulic conductivity, and of porosity. In connection with a **Monte-Carlo-procedure** stochastic simulation enables the investigation of uncertainty in parameters by analysing many equally probable, independent realizations of random fields. Given the parameters of one realization, **physical processes** like flow or solute transport can be simulated for given initial and boundary conditions by deterministic model-

ling. The outcome of such simulation are dependent variables like specific flux $\mathbf{q}(\mathbf{x})$, flow velocity $\mathbf{u}(\mathbf{x})$, piezometric head $h(\mathbf{x})$, statistical moments of a tracer cloud etc. The statistics of the variable (mean and variance) at any location \mathbf{x} characterizes the **uncertainty**. An **example** for the stochastic simulation using a Monte-Carlo technique is the generation of many fields of hydraulic conductivity K for a given flow domain. For each realization the flow field is calculated and the piezometric head $h(\mathbf{x})$ is evaluated at discrete locations. The statistical analysis yields estimates of mean, variance, covariance, and probability density function of $h(\mathbf{x})$. More general, **Monte-Carlo type simulations** can be characterized by:

- Various classes of parameters can be uncertain.
- The probability density has to be given or has to be assumed.
- For each parameter a random value is determined according to the probability density function.
- The variance of the parameter needs not necessarily to be small.
- The values of the parameters may be uncorrelated or may be correlated by given covariance functions.
- The generation process of the parameters can be conditioned by honouring measured data at discrete locations.
- For each generated parameter field the flow and transport problem is numerically solved.
- This yields a result field (e. g., piezometric head $h(\mathbf{x})$).
- Modelling is performed for each generated parameter field.
- The results are statistically evaluated (if possible mean, variance, covariance, probability density function, confidence intervals etc.) thus characterizing uncertainty.

Compared to analytical stochastic methods (e.g., Gelhar und Axness, 1983; Dagan 1989; Gelhar, 1993) Monte-Carlo techniques are more versatile and more general. However, **limits** must be mentioned. The computer memory available and the computing time may represent limits. Due to fine numerical discretisation needed the demand for computing power may increase drastically. In any case we have to ask if the numerical solution is precise enough, or if the ensemble mean does converge to the exact solution, which is not known. Furthermore the number of necessary realizations is not always clear.

In the past Freeze (1975) generated one-dimensional uncorrelated fields of hydraulic conductivity K for a given probability density function. Smith und Freeze (1979) generated two-dimensional correlated, isotropic and anisotropic fields and discussed the influence of variability in K and the boundary conditions on the variability in the piezometric head h . Ababou et al. (1989) generated three-dimensional correlated, isotropic and anisotropic fields of hydraulic conductivity K and solved the flow equation. Delhomme (1979) generated two-dimensional, correlated conditional transmissivity fields using the turning bands Method, and using kriging.

1.4.1 Conditional stochastic generation of correlated random fields

How can random fields $Z(\mathbf{x})$ be conditioned by honouring $Z(\mathbf{x}_i)$ measurements at discrete locations? This problem can be illustrated at the practical example of the generation of a ran-

dom field of hydraulic conductivity $K(\mathbf{x})$ given the variogram $\gamma_Z(\mathbf{s})$ and given K -values from short range pumping tests at various locations. Delhomme (1979) suggests the following procedure (Fig. 8).

1. A first estimate of the field $Z^*(\mathbf{x})$ is obtained by kriging based on the variogram $\gamma_Z(\mathbf{s})$ and the measurements.
2. An unconditional random field $Z_u(\mathbf{x})$ is generated based on given mean μ_Z , variance σ_Z^2 and the covariance function $R_{ZZ}(\mathbf{s})$.
3. From the field $Z_u(\mathbf{x})$ pseudo-measurements $Z_u^*(\mathbf{x}_i)$, $i=1,\dots,n$ are taken at all measurements locations \mathbf{x}_i .
4. A field $Z_p(\mathbf{x})$ is interpolated using kriging based on the pseudo-measurements $Z_u^*(\mathbf{x}_i)$, $i=1,\dots,n$. The residuum field $Z_r(\mathbf{x})= Z_u(\mathbf{x})- Z_p(\mathbf{x})$ is calculated. This residuum is considered as error estimate of $Z_p(\mathbf{x})$.
5. The residuum field $Z_r(\mathbf{x})$ is added to $Z^*(\mathbf{x})$ by $Z_c(\mathbf{x})=Z^*(\mathbf{x})+Z_r(\mathbf{x})$. This yields a conditional random field $Z_c(\mathbf{x})$ honouring the measurements as well as the variogram of $Z(\mathbf{x})$.

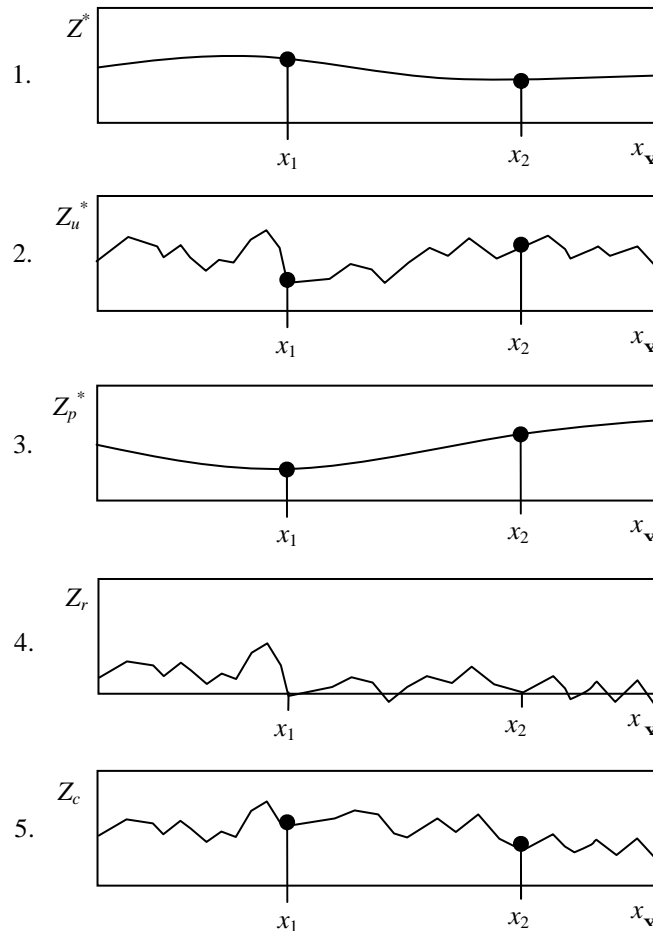


Fig. 8 Conditional stochastic simulation (schematically): 1. kriging with measurements; 2. unconditional random field; 3. pseudo-measurements, interpolated by kriging; 4. residuum; 5. conditional random field.

1.4.4 Example for stochastic modelling: Catchment of a pumping well

The application of stochastic modelling is presented for the example of the catchment of a pumping well. A simple rectangular unconfined aquifer of size 2000m×1200m is considered here. At the southern boundary a fixed head boundary condition $h=10\text{m}$ is applied. The remaining boundaries are impermeable. The flow is at steady state. The hydraulic conductivity K is 432 m d^{-1} and the recharge rate is $N=1\text{mm/d}$. The well is located 995m from the western boundary and 505 from the southern boundary. The pumping rate is $432\text{m}^3\text{d}^{-1}$. The random K -fields are unconditional and is characterized by a geometric mean of 5mm/s , and an exponential covariance function $R_Y(s)$ with variance σ_Y^2 of 1, and a correlation length l_Y of 100m. The K -fields and the catchment of two realizations together with the corresponding piezometric head field are shown in Fig. 9. The two catchments exhibit considerable differences. The ensemble of a total of 1000 realization was statistically evaluated (Fig. 10). The figure shows the probability of a water particle at a particular location to reach the well. (Stauffer et al., 2002). The boundary with probability 0.5 corresponds to the catchment for homogeneous K with high accuracy. Stauffer et al. (2002) and Stauffer (2005) developed a semi-analytical theory for a fast assessment of the uncertainty of the boundary of the well catchment.

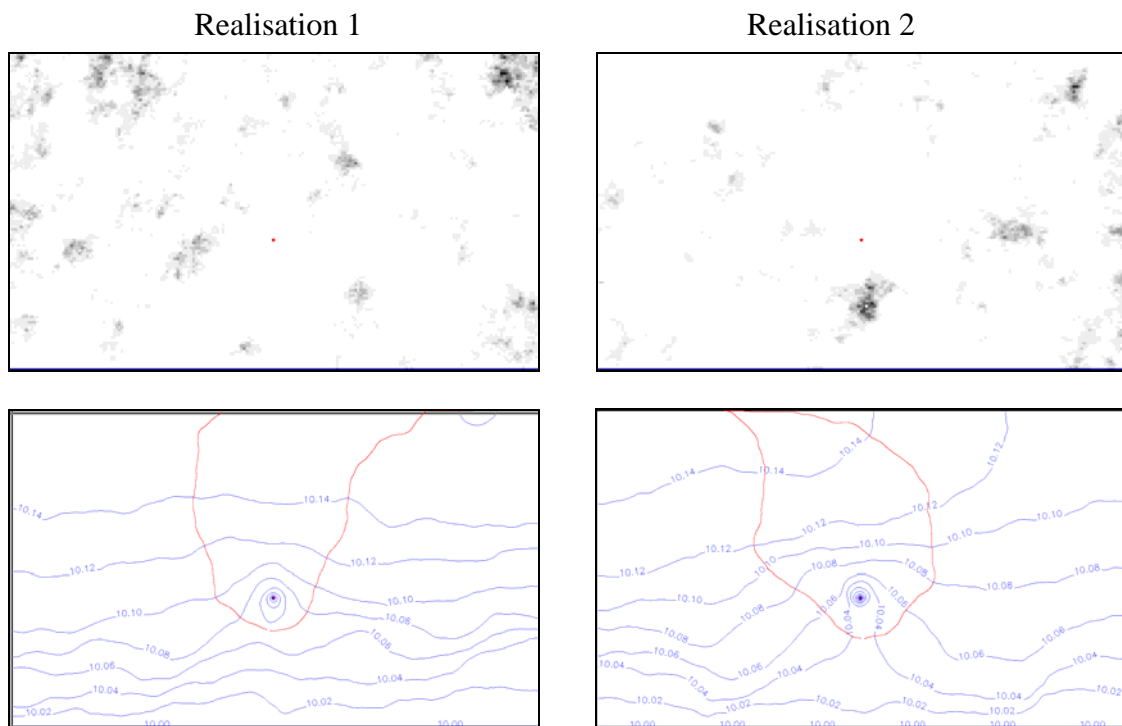


Fig. 9 Stochastic simulation of the catchment of a pumping well: Top: Two unconditional realizations of hydraulic conductivity fields (dark areas are high permeability and bright areas are low permeability zones); bottom: piezometric head and well catchment (red).

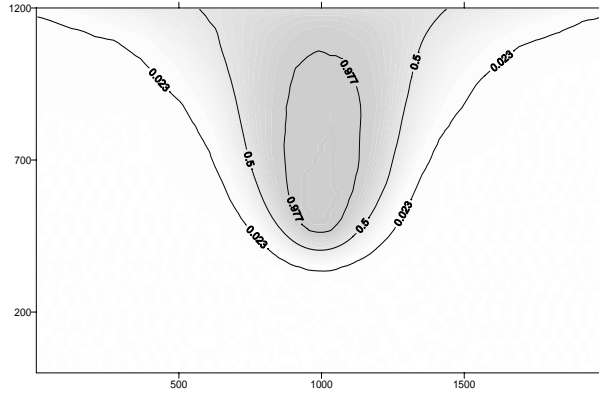


Fig. 10 Stochastic simulation of the catchment of a pumping well: Statistical evaluation of 1000 unconditional realizations of hydraulic conductivity fields with indication of the probability of a water particle to belong to the well catchment.

1.5 Effective flow parameters

1.5.1 Saturated flow parameters

Let's start with the more general term '**equivalent parameter**'. In general a complex system is described by one or several equivalent parameters of functions in simplified manner. In the case of a heterogeneous aquifer an equivalent is related to a homogeneous replacing medium with (at least zone-wise) homogeneous properties. Such parameters have to fulfil specific conditions. Usually it is required for hydraulic conductivity that the flux across the boundary is identical for given hydraulic head at the boundary in both the heterogeneous and the homogeneous system. Obviously, equivalent parameters only characterize a specific average behaviour. With respect to saturated porous media we concentrate on hydraulic conductivity $K(\mathbf{x})$. Starting point is local validity of Darcy's law.

We may consider averaging of Darcy's law over a control volume. By postulating a **generalized Darcy's law** for the average according to:

$$\langle \mathbf{v} \rangle = -\mathbf{K}_{\text{eq}} \nabla \langle h \rangle \quad (2)$$

includes the concept of an **equivalent hydraulic conductivity** \mathbf{K}_{eq} . The question arises whether equivalent parameters exist, which depend only on the porous medium and its heterogeneous structure, and not on further parameters like flow conditions, boundary condition, or time.

A stochastic approach consists of considering mean uniform flow in a infinite stationary heterogeneous aquifer (Dagan, 1989). Usually it is assumed that hydraulic conductivity $K(\mathbf{x})$ is locally isotropic and log-normally distributed, and fulfils an isotropic or anisotropic covariance function $R_Y(\mathbf{s})$ with $Y = \ln(K)$ with the parameters variance and correlation length. For such conditions it is possible to perform an averaging process over the ensemble of all possible realizations, and to establish a relation between expectation $E[\mathbf{q}] = \langle \mathbf{q} \rangle$ and $E[h] = \langle h \rangle$ (Dagan, 1989):

$$\langle \mathbf{v} \rangle = -\mathbf{K}_{\text{eff}} \nabla \langle h \rangle = -\mathbf{K}_{\text{eff}} \mathbf{I}$$

The parameter \mathbf{K}_{eff} is called **effective hydraulic conductivity**. It is valid for the specific conditions mentioned above. For an infinite domain the ensemble average can be replaced by the spatial average according to the ergodicity hypothesis. In this context $K_{\text{eq}}=K_{\text{eff}}$ in equation 2 . This implies in practice that the domain has to be large enough with respect to the correlation length of Y . Furthermore, an **averaged balance equation**, averaged over all realizations can be formulated (Dagan, 1989):

$$S_{\text{eff}} \frac{\partial \langle h \rangle}{\partial t} = \nabla \cdot (\mathbf{K}_{\text{eff}} \nabla \langle h \rangle) \quad (3)$$

S_{eff} is the effective specific storativity. Again the remarks hold concerning ergodicity. Equation 3 is formally identical to the flow equation for homogeneous conditions.

In the following some **results from stochastic theories** for steady flow in an infinite domain of a non-compressible fluids are presented and discussed.

For **one-dimensional flow** K_{eff} corresponds to the **harmonic mean** K_{harm} for all kinds of heterogeneities without restriction concerning flow geometry. For log-normally distributed and stationary K the effective conductivity is (Gelhar, 1993):

$$K_{\text{eff}} = K_g \exp\left(-\frac{\sigma_Y^2}{2}\right)$$

The parameter K_g is the geometric mean of K . The result is independent of the correlation length of Y .

For **two-dimensional, uniform mean flow** K_{eff} corresponds to the geometric mean K_g after Matheron (de Marsily, 1984) for log-normally distributed K , assuming local isotropy. The result is valid for isotropic covariance functions of any kind. Therefore it is independent from variance σ_Y^2 and correlation length l_Y . The result can be used for isotropic transmissivity fields as well.

For **three-dimensional flow** first order approximations exist for expressing K_{eff} for log-normal K and isotropic as well as anisotropic covariance functions $R_Y(s)$ with isotropy in the horizontal plane (Dagan, 1989, Gelhar, 1993), but also second order corrections (Dagan, 1993, Indelman und Abramovich, 1994). Neuman and Orr (1993) suggest a formulation for the \mathbf{K}_{eff} tensor. Further theoretical and empirical approaches can be found in Renard and de Marsily (1997). For cases with arbitrary probability density function the following approximation might be useful (‘Self-consistent approach’ according to the theory of embedded matrix, Dagan, 1989):

$$K_{\text{eff,hor}} = \frac{1}{2 \int_0^{\infty} \frac{f(K)}{(K - K_{\text{eff,hor}}) \mu(\varepsilon) + 2K_{\text{eff,hor}}} dK}$$

$$\mu(\varepsilon) = \frac{\varepsilon^2}{1 - \varepsilon^2} \left(\frac{1}{\varepsilon \sqrt{1 - \varepsilon^2}} \cdot \text{arctg} \left(\sqrt{\frac{1}{\varepsilon^2} - 1} \right) - 1 \right)$$

$$\varepsilon = \frac{\lambda_{\text{vert}}}{\lambda_{\text{hor}}} \sqrt{\frac{K_{\text{eff,hor}}}{K_{\text{eff,vert}}}}$$

$$K_{\text{eff,vert}} = \frac{1}{\int_0^{\infty} \frac{f(K)}{(K_{\text{eff,hor}} - K) \mu(\varepsilon) + K} dK}$$

The result is again valid for anisotropic random fields with isotropy in the horizontal plane. Moreover it is not limited to small variances σ_Y^2 . Again local isotropy of K is assumed. The evaluation of K_{eff} using the above equations has to be performed iteratively.

How is the situation for non-uniform mean flow as in the case of radial flow? For **plane radial flow** to a well the effective hydraulic conductivity corresponds to the harmonic mean near the well. Neuman und Orr (1993) showed with the help of Monte Carlo simulations that in a sufficient distance from the well the geometric mean is valid. The **radial mean flow** to a complete well in three-dimensional confined heterogeneous aquifer was investigated by Indelman et al. (1996). The heterogeneity corresponded to a three-dimensional anisotropic random field of $Y=\ln(K)$. They observed that the concept of an effective hydraulic conductivity is not well suited for practical application. They postulated an equivalent hydraulic conductivity according to the well function after Theis depending on pumping rate, distance from the well, and mean piezometric head. They showed by a stochastic analysis that near the well K_{eff} corresponds to the arithmetic mean. Far away from the well the K_{eff} for uniform mean flow is valid, depending on the ratio between vertical to horizontal correlation length. Therefore the concept of effective hydraulic conductivity depends here on the flow geometry.

The **influence of boundaries and of transient flow** on K_{eff} was discussed by Dagan (1989) and others. Accordingly the influence of a boundary of the flow domain is restricted to a relatively small region along the boundary. For transient flow K_{eff} is also transient. Nevertheless, it approaches K_{eff} for steady flow relatively soon. Therefore the generalized Darcy law with $K_{\text{eq}}=K_{\text{eff}}$, does represent an approximation also for weakly non-uniform and transient flow.

For general **transient, non-uniform mean flow** in stationary random fields of $Y=\ln(K)$ Indelman und Abramovich (1994) postulate a **non-local concept of effective hydraulic conductivity** $\mathbf{K}_{\text{eff}}(\mathbf{x}, \mathbf{x}')$ together with a convolution integral. This parameter reduces to \mathbf{K}_{eff} for uniform mean flow. For conditional hydraulic conductivity fields Neuman und Orr (1993) also proposed a non-local concept.

In practical applications it is not always possible to adopt effective hydraulic conductivity parameters. An alternative can be the formulation of **block hydraulic conductivity** values $\mathbf{K}_{\text{Block}}$ (see, e. g., Renard and de Marsily, 1997) according to the numerical discretisation. Such block values are considered constant within a limited domain, the block, which may

show non-stationary behaviour. In the limit of very large blocks $\mathbf{K}_{\text{Block}}=\mathbf{K}_{\text{eff}}$. Various methods exist for the estimation or determination of block hydraulic conductivity values by **upscaling** (Sanchez-Vila et al., 1995; Renard and de Marsily, 1997; Attinger 2002). The resulting parameter may be a non-symmetric tensor.

The parameters **effective specific storativity** $S_{0,\text{eff}}$ and **effective storativity** S_{eff} can approximately be described by the arithmetic mean storativity (Dagan, 1989).

1.6 Effective transport parameters

The local mass balance for a solute without source and sink term is:

$$\frac{\partial(nc)}{\partial t} + \nabla \cdot [c \mathbf{v}] - \nabla \cdot [n \mathbf{D}_h \nabla c] = 0$$

Expressing the stochastic variables concentration $c(\mathbf{x},t)$ and velocity $\mathbf{u}(\mathbf{x},t)$ by ensemble mean and perturbation:

$$\begin{aligned} c(\mathbf{x}, t) &= \langle c(\mathbf{x}, t) \rangle + c'(\mathbf{x}, t) \\ \mathbf{u}(\mathbf{x}, t) &= \langle \mathbf{u}(\mathbf{x}, t) \rangle + \mathbf{u}'(\mathbf{x}, t) \end{aligned}$$

the transport equation is for constant porosity n and local dispersion coefficient \mathbf{D}_h :

$$\frac{\partial(\langle c \rangle + c')}{\partial t} + \nabla \cdot [(\langle c \rangle + c') \cdot (\langle \mathbf{u} \rangle + \mathbf{u}')] - \mathbf{D}_h \nabla^2 (\langle c \rangle + c') = 0$$

Taking the ensemble mean leads to:

$$\frac{\partial \langle c \rangle}{\partial t} + \nabla \cdot (\langle \mathbf{u} \rangle \langle c \rangle) - \nabla \cdot (\langle \mathbf{u}' c' \rangle) - \mathbf{D}_h \nabla^2 \langle c \rangle = 0$$

The third and the fourth term are usually written according to a Fickian approach. The ensemble mean equation reads:

$$\frac{\partial \langle c \rangle}{\partial t} + \nabla \cdot (\langle \mathbf{u} \rangle \langle c \rangle) + \nabla \cdot (\mathbf{D}_{\text{eff}}(t) \nabla \langle c \rangle) = 0$$

The coefficient $\mathbf{D}_{\text{eff}}(t)$ is the effective dispersion coefficient, with:

$$\mathbf{D}_{\text{eff}}(t) = \mathbf{D}_h + \langle \mathbf{u} \rangle \mathbf{A}(t)$$

The coefficient $\mathbf{A}(t)$ is the macrodispersivity tensor.

1.6.1 Asymptotic macrodispersivity

Consider a uniform mean saturated flow in a infinite domain characterized by an anisotropic covariance function of $Y=\ln(K)$, and an instant injection of a tracer a location. What is

the expected asymptotic dispersion coefficient after sufficiently long travel distance or travel time?

For the **asymptotic longitudinal macrodispersivity** Dagan (1988) and Neuman et al. (1987) present first order approximation for an exponential covariance function of $R_Y(\mathbf{s})$:

$$A_l = \sigma_Y^2 I_Y$$

The parameter I_Y is the horizontal correlation length of Y . The result is valid for a high Peclet-number according to:

$$Pe = \frac{v \cdot I_Y}{D_l} = \frac{I_Y}{a_l}$$

The results correspond also to a pure advective transport of a tracer cloud without local dispersion. Therefore, a large enough initial volume is required in order to get spreading of the plume. Neuman et al. (1987) investigated the influence of local dispersion on A_l .

After Gelhar und Axness (1984) and Dentz et al. (2000) the asymptotic longitudinal macrodispersivity is for horizontal flow and high Peclet-number partly differs:

$$A_l = \frac{\sigma_Y^2 \cdot I_Y}{\gamma^2}$$

The factor γ is called flow factor:

$$\gamma = \frac{v}{i_x \cdot K_g} = \frac{K_{eff}}{K_g}$$

where K_{eff} is the effective hydraulic conductivity and i_x is the hydraulic gradient in the mean flow direction. For two-dimensional flow $\gamma=1$. Moreover, for very small variance σ_Y^2 the factor γ is practically one.

The difference lies in different consideration of terms in the theoretical development of the approximation. Anyhow, the results are valid only for small variance σ_Y^2 . For higher variances non-linear effects are expected.

The asymptotic transversal macrodispersivity A_t is small compared to local transversal dispersivity a_t , and therefore can be neglected. The results are again valid only for small variance σ_Y^2 .

1.6.2 Temporal development of macrodispersivity

Again, an ideal tracer of mass M is locally injected in an infinite, uniform mean flow field. The covariance function $R_Y(\mathbf{s})$ is anisotropic and is characterized by the horizontal and the vertical correlation lengths $I_{Y,hor}$ and $I_{Y,vert}$. Regarding the ensemble of the tracer cloud at a given time the following situations be distinguished (Fig. 11):

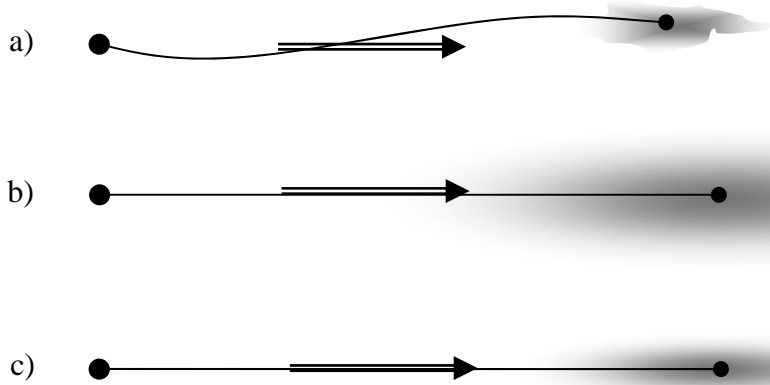


Fig. 11 Tracer distribution of an initially locally injected tracer mass after transport time; a) for a single realization; b) for the ensemble mean; c) for the ensemble mean relative to the centre of mass (black dots) of single realizations.

For the temporal **development of the ensemble mean mass distribution** (second moment of the particle displacement) according to Fig. 11 a) Dagan (1988) formulated first order approximations for a purely advective transport. The results can be presented as apparent macrodispersivity $A_{app}(t)=M/(2U)$ over transport time or mean transport distance (Fig. 12-14), where M is the second moment. The apparent macrodispersivity A_{app} is a parameter value for transport simulation using constant $A(t)$ for a given transport time, and therefore is also dependent on time or mean transport distance. For deterministic transport modelling the concept of an apparent macrodispersivity is useful and enables relatively simple solutions for transport problems in heterogenous aquifer.

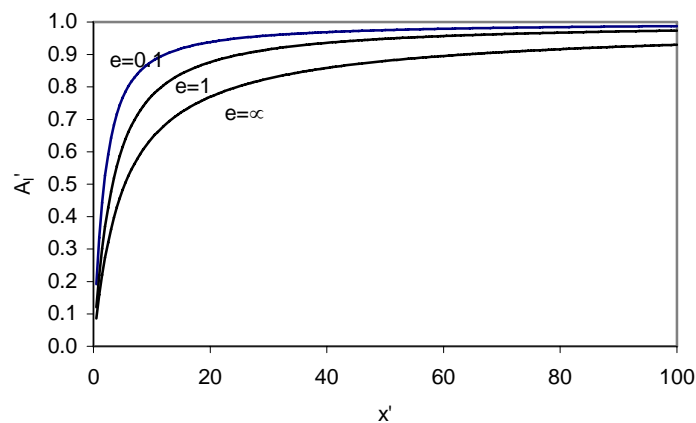


Fig. 12 Development of the apparent longitudinal macrodispersivity $A_l'(x')=A_{l,app}(x)/A_{l,asympt}$ with $x'=x/l_{hor}$ for anisotropic random variable $Y=\ln(K)$ for various ratio e of vertical to horizontal correlation length (after Dagan, 1989).

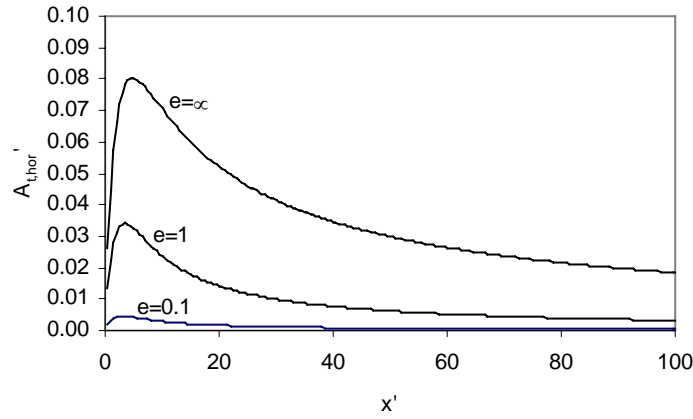


Fig. 13 Development of the apparent transversal horizontal macrodispersivity $A_{t,hor}'(x')=A_{t,hor,app}(x)/A_{t,asympt}$ with $x'=x/I_{hor}$ for anisotropic random variable $Y=\ln(K)$ for various ratio e of vertical to horizontal correlation length (after Dagan, 1989).

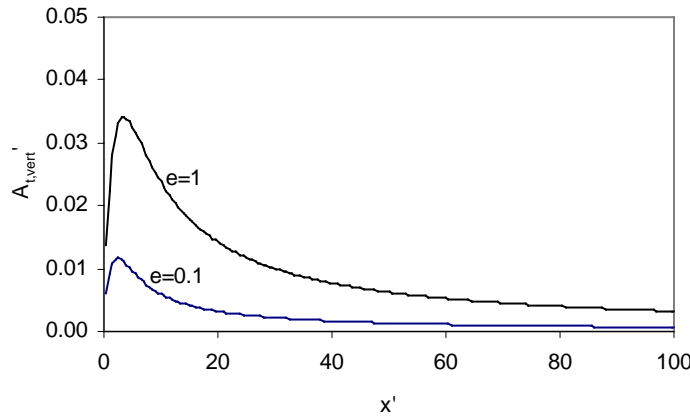


Fig. 14 Development of the apparent transversal vertical macrodispersivity $A_{t,vert}'(x')=A_{t,vert,app}(x)/A_{t,asympt}$ with $x'=x/I_{hor}$ for anisotropic random variable $Y=\ln(K)$ for various ratio e of vertical to horizontal correlation length (after Dagan, 1989).

The temporal development of the ensemble mean mass distribution was investigated by Dentz et.al. (2000) for a Gaussian covariance function R_Y . They developed expressions for the time-dependent effective macrodispersivity $A(t)=1/(2U)dM(t)/dt$. As indicated in Fig. 11c) the second moment of the mass centre related mass distribution is generally smaller than the ensemble mean distribution. However, in the asymptotic case they get identical.

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