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Estimating aquifer transmissivities — on the value of auxiliary data

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Abstract

Groundwater quality modelling relies heavily on the knowledge of preferential flowpaths such as buried stream channels and their distribution within the aquifer. This paper examines the extent to which these patterns may be identified by including auxiliary data, such as transverse electric resistances or specific capacities, when estimating the transmissivity field. The analyses are based on two hypothetical aquifers. The first involves a high transmissivity flowpath. The second is a realization of a correlated random field with the same spatial moments as the organised case. Monte Carlo simulations and cokriging estimates are used to analyse the effect of the number of samples and their correlation with transmissivity on the width of the capture zone of a well. Results indicate that, in the organised case with no auxiliary information, the estimated widths are substantially biased. This bias can be reduced significantly by including auxiliary data, even when poorly correlated to transmissivity. Auxiliary data also reduce the scatter (i.e. standard deviation) of the estimated widths significantly, which is a measure of the accuracy of the estimates. In the example used here, 70 samples of auxiliary data, which are correlated to transmissivity by $r = 0.6$, outweigh the information from 12 additional pumping tests. For the case of the correlated random field, the benefit of using auxiliary data is much less pronounced both in terms of removing the bias and in terms of accuracy (i.e. standard deviation). It is concluded that auxiliary data are useful for estimating transmissivity fields in the context of groundwater quality modelling, particularly when channelised flow is to be expected.

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1. Introduction

It is now widely being recognised that (lack of) ability to determine accurate hydraulic conductivity distributions is one of the major limitations on groundwater quality modelling (Sudicky and Huyakorn, 1991). Specifically, it has been shown that a knowledge of pathways and their distribution is of much greater importance for solute transport than an evaluation of effective parameters (Silliman and Wright, 1988). Indeed, Williams (1988) and Anderson (1991) criticised the common assumption of random media properties (e.g. Neuman, 1990) and emphasised the presence of organised discrete units as formed by geological processes. Williams (1988) also pointed out that the apparent disorder is largely a consequence of studying the subsurface through point measurements such as boreholes. These ideas have recently stimulated exciting research into the effects of organisation in aquifers and catchments (e.g. Ritzi and Dominic, 1993; Blöschl et al., 1993; Blöschl and Sivapalan, 1995).

Unfortunately, model calibration based on groundwater heads can provide effective transmissivities, but is notoriously poor in identifying realistic patterns of pathways (Blaschke, 1991; Mackay and Riley, 1991). Breakthrough curves of conservative tracers are ideal for setting up transport models but are virtually never available in practical cases. Similarly, obtaining a large number of transmissivities 'directly' is usually prohibited by the enormous costs associated with pumping tests.

As a way out of this dilemma, it has been suggested that 'auxiliary information' is used to enhance the estimation of conductivity or transmissivity fields. Auxiliary data such as transverse electric resistances or specific capacities are very inexpensive and can therefore be obtained at many points within the domain of interest. Moreover, they are potentially capable of identifying patterns of preferential pathways such as buried stream channels. However, these auxiliary data are often poorly correlated with transmissivity. Little is known about the benefit of large a amount of auxiliary data, given the poor correlation. The objectives of this paper are (a) to assess the relative importance of the number of auxiliary data versus their correlation with transmissivities and (b) to compare the effect of organisation and randomness in the underlying transmissivity field.

Potential candidates for auxiliary data in groundwater modelling are electric transverse resistances, seismic data and specific capacities. Ahmed and de Marsily (1987) analysed 56 transmissivities and specific capacities for an aquifer in northern France and arrived at a correlation coefficient of 0.87. Mazáč et al. (1985) discuss the factors affecting the relationship between electric and hydraulic properties of aquifers. For example, increased clay content tends to decrease both electric resistivities and hydraulic conductivities. However, their data show poorly defined relationships. Frohlich and Kelly (1985) present data of transmissivities and electric transverse resistances corresponding to correlation coefficients (r) as high as 0.9. A field study in lower Austria (Kupfersberger et al., 1992), however, yielded much lower correlation coefficients. The area analysed was 3 km^2 in size and comprised highly heterogeneous fluvial deposits, with grain sizes ranging from sand to gravel, and clay lenses. For this aquifer, correlation coefficients between transverse electric resistances and transmissivities were of the order of 0.4–0.5. These values are much lower than those obtained by Frohlich and Kelly (1985). This may well be because Frohlich and Kelly analysed five points only while the Austrian study comprised 32 data pairs.

In this paper, three cases of the correlation between generic auxiliary data and transmissivities ($r = 0.4$, 0.6 and 0.8) are analysed and compared with the case of perfect correlation ($r = 1.0$). Perfect correlation is used to represent the information ideally provided by additional pumping tests. This allows determination of the number of pumping tests ($r = 1.0$) that can be saved by performing geophysical measurements ($r < 1.0$).

Methods of incorporating auxiliary data for estimating aquifer transmissivities are invariably based on the scenario of a few transmissivities and on the availability of many auxiliary data. The basic idea of these methods is to infer the transmissivities at undersampled points from auxiliary data at those points. A recent contribution to incorporating geophysical data is given by Rubin et al. (1992) who developed a geophysical hydrogeological inverse model using seismic data. In practical cases, much simpler regression models are used (e.g. de Marsily, 1986). An alternative and more elaborate method is cokriging. Cokriging is a linear estimation technique for estimating two (or more) correlated variables. Central to this technique are the variograms that describe the correlation structure of the variables. These are usually derived from measurements. Specifically, one limiting requirement is that the two variables have a sufficient number of common data points for inferring reliable cross-variograms. This is not always possible. For example, metal tubes in wells may disallow the taking of electric resistance soundings in the immediate vicinity.

The advantage of cokriging over other estimation techniques has been demonstrated by a number of authors (e.g. Ahmed and de Marsily, 1987). Aboufirassi and Mariño (1984) used cokriging to construct maps of transmissivity with measurements of transmissivity and specific capacity while Ahmed et al. (1988) used cokriging with electrical properties as auxiliary variables. This paper follows that paradigm.

2. Method

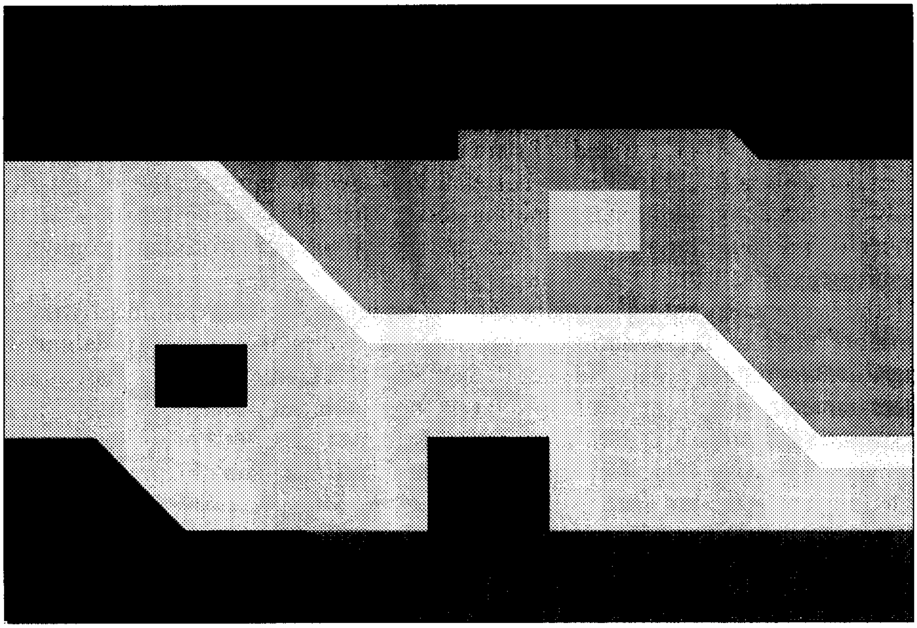
2.1. Cokriging theory

Consider two second order stationary random functions $Z(x_i)$, $i = 1, \ldots, n$ and $Y(x_j), j = 1, \ldots, m$, with $n < m$ (i.e. undersampled case), under the intrinsic assumption. Cokriging assumes that the estimated Z value at any point x_0 is a linear combination of the measurements:

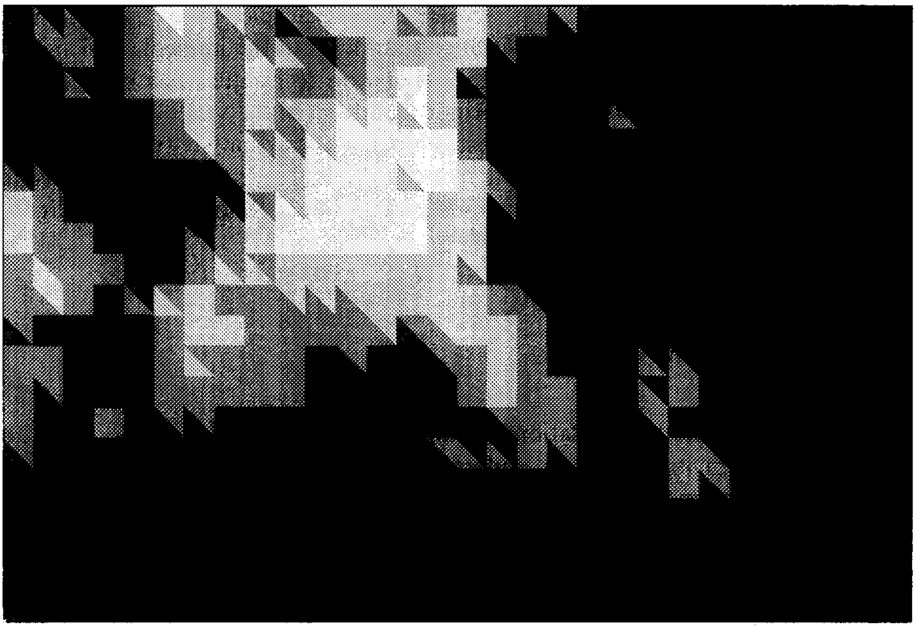
$$Z^*(x_0) = \sum_{i=1}^{n} \lambda_i Z(x_i) + \sum_{j=1}^{m} \nu_j Y(x_j) \tag{1}$$

The unknown coefficients λ_i and ν_j are determined by the following two conditions. First, the estimates are required to be unbiased

$$E[Z(x_0) - Z^*(x_0)] = 0 \tag{2}$$



(a)



(b)

Fig. 1. Transmissivity distributions of the hypothetical aquifers. Values range from 100 (dark areas) to 6000 m^2 day^{-1} (light areas). (a) Organised transmissivity distribution; (b) realisation of a correlated random field as used in this study. The size of the domain is 6000 m by 4000 m.

where E denotes the expectation. Second, the estimates are required to be 'optimal' in the sense that the variance of the estimation error is to be minimal

$$\mathrm{var}[Z(x_0) - Z^*(x_0)] = \text{minimum} \tag{3}$$

Application of Lagrange multipliers results in a cokriging system which can be written in matrix form as

$$\mathbf{A} \cdot \boldsymbol{X} = \boldsymbol{B} \tag{4}$$

The matrix **A** consists of the spatial correlation of the two variables and their cross-correlation. The vector $\boldsymbol{B}$ contains the relative geometric condition of the point x_0 to be estimated and the points where a datum is observed. $\boldsymbol{X}$ is the solution vector of the kriging weights λ_i and ν_j. More detailed information is provided by Journel and Huijbregts (1978), Myers (1982), Aboufirassi and Mariño (1984) and Wackernagel (1993).

2.2. Set-up of hypothetical aquifer

Fig. 1 shows the transmissivity distributions of the two hypothetical aquifers used in this study. The first aquifer (Fig. 1(a)) is referred to as the organised case. The transmissivity pattern consists of a high permeability flowpath representing a buried stream channel. Transmissivities decrease towards the upper and lower boundary of the domain as is typical of aquifers in Alpine valleys. Several local inhomogeneities

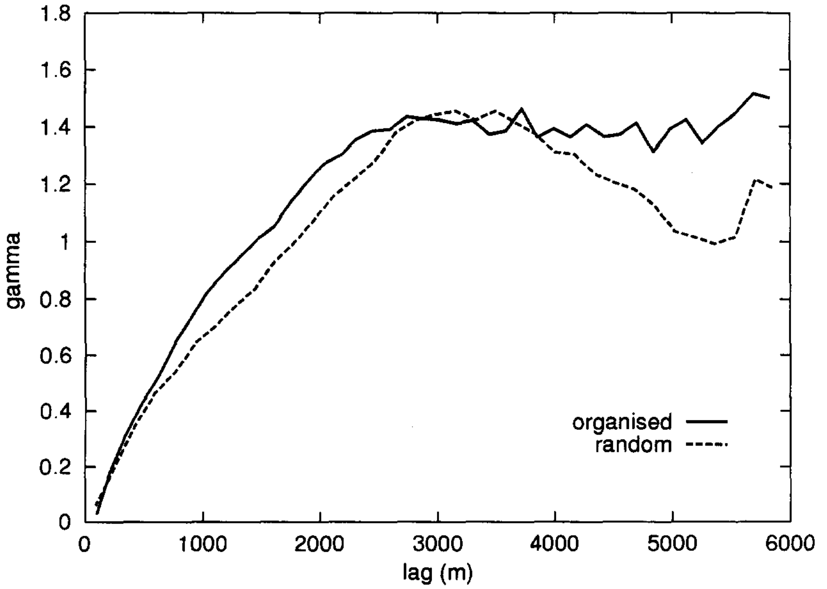


Fig. 2. Empirical variograms for the organised (solid line) and the random (dashed line) transmissivity distributions of Fig. 1.

are included. The implications of this type of heterogeneity on groundwater modelling and its relation to geology are discussed in more detail by Blaschke (1990).

The second aquifer (Fig. 1(b)) is referred to as the random case and is a realisation of a correlated random field. The random field was generated as an unconditional simulation with the same mean (7.0) and standard deviation ($\sigma = 1.1$) of the logarithms of transmissivity as the organised case. The turning bands method (Mantoglou and Wilson, 1982) was used. The semivariograms for the organised and the random case are given in Fig. 2. The two semivariograms are clearly very similar.

2.3. Generating auxiliary data

For each simulation run, auxiliary data within the domain are generated by

$$\log(\text{aux}) = \log(T) + \epsilon \tag{5}$$

where T denotes the transmissivity and aux denotes the auxiliary variable. The error ϵ is assumed to be statistically independent of T, uncorrelated in space and Gaussian distributed (i.e. $N(0, \sigma_\epsilon)$) with

$$\sigma_\epsilon = \sqrt{1 - r^2}\,\frac{1}{r}\,\sigma_T \tag{6}$$

where r is the correlation coefficient (in the logarithmic space) and σ_T denotes the standard deviation of log (T) (Sachs, 1974). In this study, the cases $r = 0.4$, 0.6, 0.8 and 1.0 are analysed.

Table 1
Parameters in the logarithmic space for the variograms and cross-variograms for various correlation coefficients r. T denotes the transmissivity and aux denotes the auxiliary variable. The range is 2700 m for all cases. The sill refers to the spherical component of the variogram only

	Nugget	Sill
$r = 1.0$		
Variogram log (T)	0.0	1.4
Variogram log (aux)	0.0	1.4
Crossvariogram	0.0	1.4
$r = 0.8$		
Variogram log (T)	0.0	1.4
Variogram log (aux)	0.7	1.4
Crossvariogram	0.0	1.4
$r = 0.6$		
Variogram log (T)	0.0	1.4
Variogram log (aux)	2.1	1.4
Crossvariogram	0.0	1.4
$r = 0.4$		
Variogram log (T)	0.0	1.4
Variogram log (aux)	6.3	1.4
Crossvariogram	0.0	1.4

2.4. Monte Carlo simulations

For each simulation run, 10 samples are drawn at random from one of the transmissivity fields (Fig. 1), and, depending on the case, 0, 5, 15, 40, 70, 110 or 190 samples are drawn from the auxiliary data field. The 10 samples from the transmissivity field represent pumping tests. The varying number of samples from the auxiliary data field represent additional (auxiliary) geophysical data. All data are transformed to the logarithmic space, used for cokriging and the resulting estimates are retransformed. Variograms are determined from the complete field rather than from a limited number of samples. With this assumption, uncertainty in the model results due to imperfectly known variogram parameters is avoided. This topic is discussed in further detail by Webster and Oliver (1993) and Wingle and Poeter (1993) among others. Spherical variograms are fitted. Nuggets and sills are given in Table 1 with the sill values referring to the spherical component of the variogram only. The range is 2700 m for all cases. These variogram values were used for both the organised and the random case.

Each of the estimated transmissivity distributions is used to drive a two-dimensional groundwater flow model (Blöschl and Blaschke, 1992) for steady state conditions. Boundary conditions (Fig. 3) consist of no flow boundaries at the top and the bottom of the domain (representing the sides of an Alpine valley), prescribed heads on the left and the right (18.3 m difference in heads), and a well with 6000 m^3 day^{-1} extraction for the organised case and 3500 m^3 day^{-1} for the random

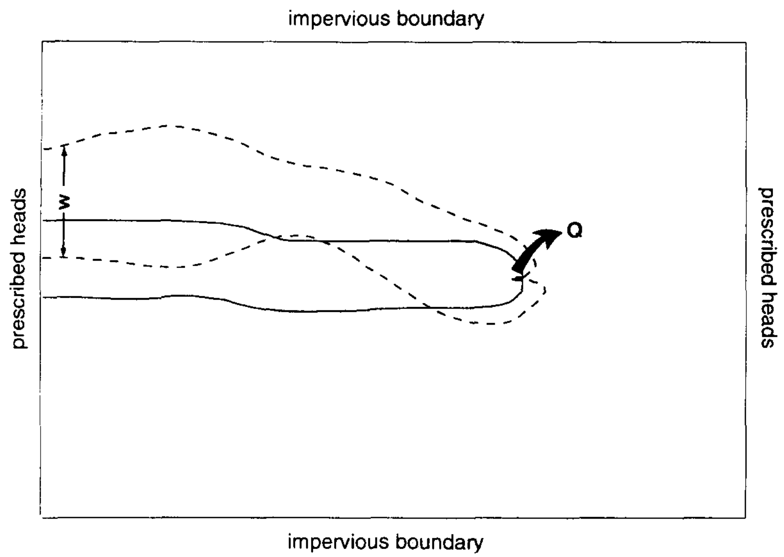


Fig. 3. Boundary conditions of the hypothetical aquifers. w denotes the width of the separating stream lines to the well. Ambient flow is from left to right. Well discharge Q is 6000 m^3 day^{-1} for the organised case and 3500 m^3 day^{-1} for the random case. Separating stream lines are shown for the organised (solid line) and the random (dashed line) case.

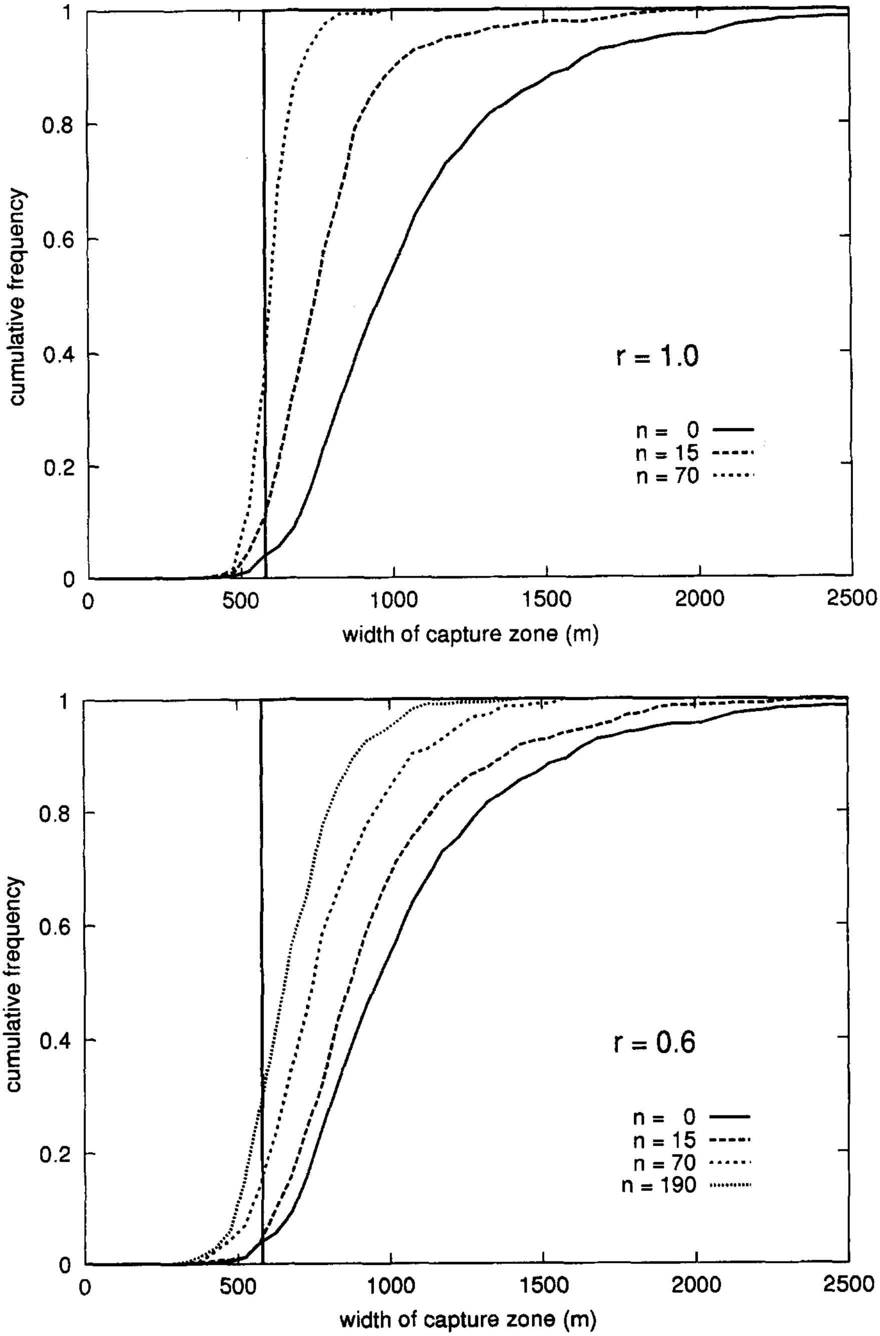


Fig. 4. Cumulative frequency distributions of the widths of the capture zone for various correlation coefficients r and number of additional samples n; the underlying transmissivity field shows organisation (Fig. 1(a)).

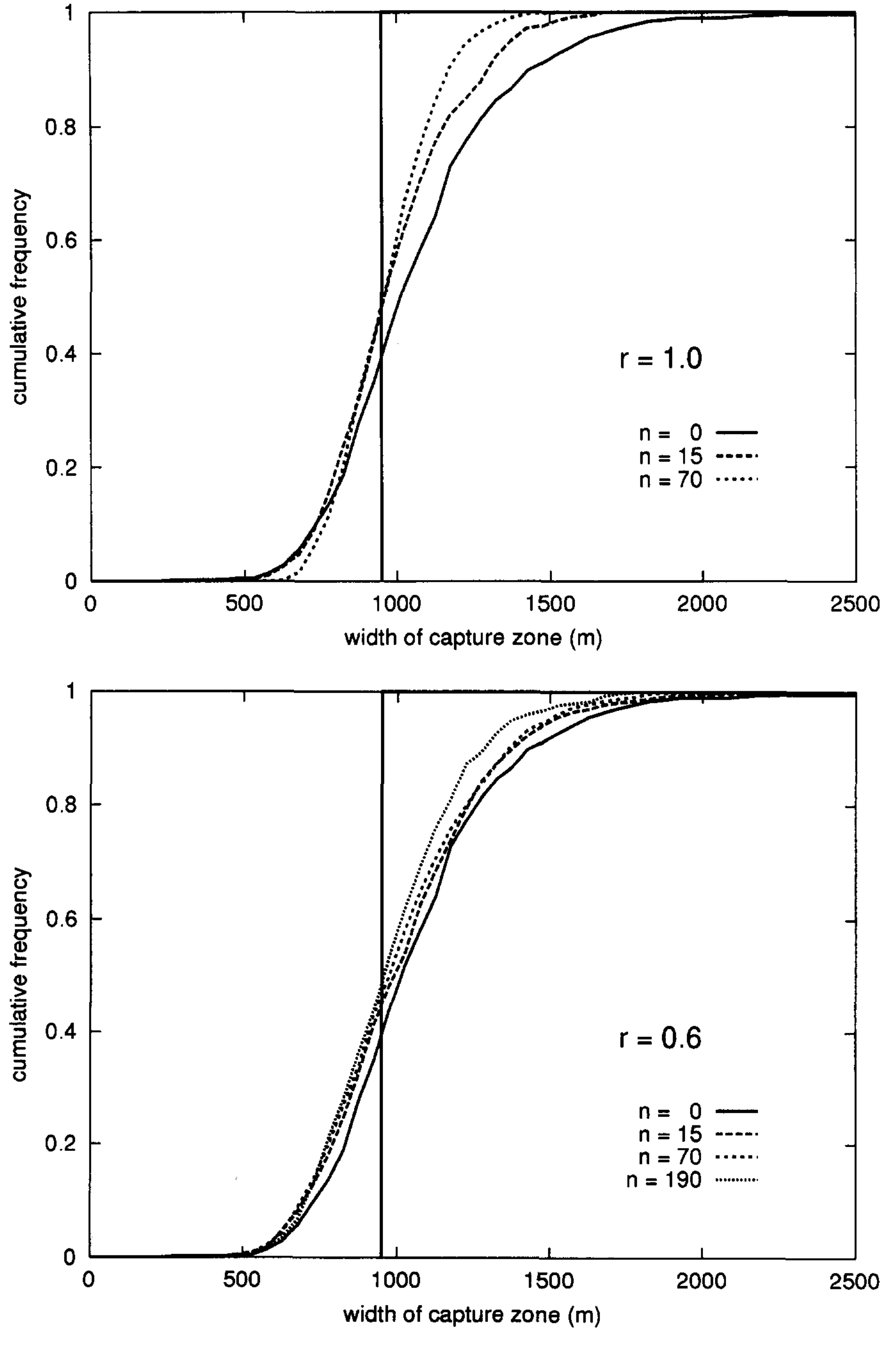


Fig. 5. Cumulative frequency distributions of the widths of the capture zone for various correlation coefficients r and number of additional samples n; the underlying transmissivity distribution is a correlated random field (Fig. 1(b)).

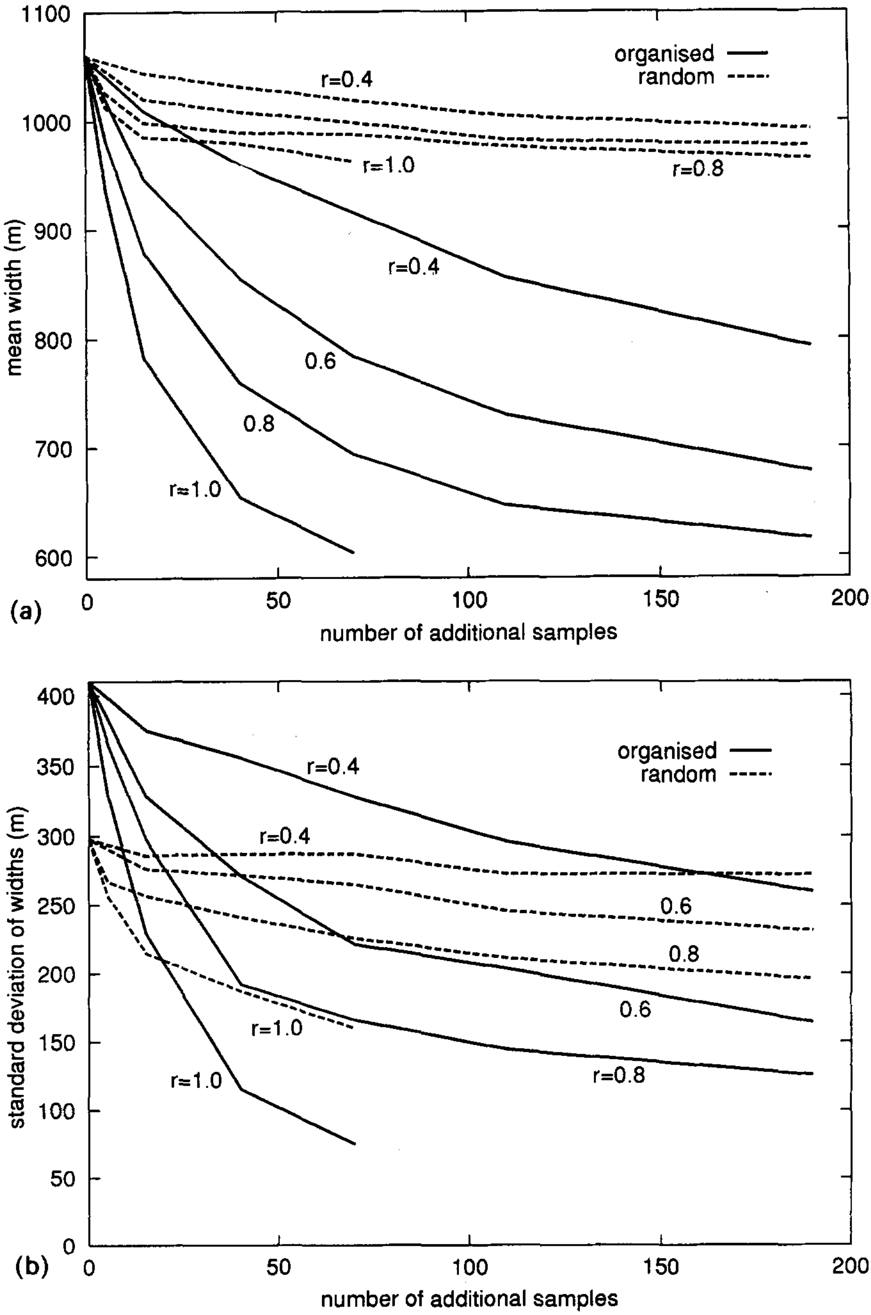


Fig. 6. (a) Mean and (b) standard deviation for the organised and the random transmissivity distributions and for various correlation coefficients r and number of additional samples n. The 'true' mean widths (Fig. 6(a)) are 580 m and 950 m for the organised and the random cases, respectively.

case. The lower extraction in the random case was selected so as not to obtain exceedingly large widths of the capture zone.

The accuracy of the transmissivity field is assessed by comparing the simulated widths of the capture zone with the true width. The capture zone to the well is defined by the separating stream lines (see Fig. 3) and the width is measured at the left boundary of the domain. This width is deemed to be an important parameter for capturing preferential flowpaths in the context of groundwater quality modelling.

For each combination of number of samples n and correlations r, 500 simulations are performed and the resulting widths are analysed statistically.

3. Results

Fig. 4 shows examples of the cumulative distribution functions of the widths of the capture zone for various number of samples ($n = 0, 15, 70, 190$) and two correlations ($r = 1.0$ and 0.6) for the organised case. The line at 580 m corresponds to the true width as obtained with the transmissivity distribution of Fig. 1(a). As would be expected, the accuracy of the estimates increases with the number of samples and correlation. Ordinary kriging with 10 transmissivities only, i.e. no auxiliary information, (solid lines in Fig. 4) yields substantially biased estimates. The mean is 1060 m. As auxiliary information is included and the number of samples increases, this bias is drastically reduced. For example, 70 additional samples of correlations 0.6 and 1.0 yield means of 780 and 600 m, respectively.

Fig. 5 displays the cumulative distribution functions of the widths of the capture zone for the random case. For this case, the true width is 950 m. Unlike the organised case there is almost no bias. 70 additional samples of correlations 0.6 and 1.0 yield means of 980 and 960 m, respectively, and these values are very close to the true value of 950 m.

For the organised case (Fig. 4), improvements in terms of the scatter around the mean (i.e. slope of the cumulative distribution function at its mean) are highly dependent on the correlation coefficient. For perfect correlation ($r = 1.0$), the improvement is large while for $r = 0.6$ it is much lower. The random case indicates a much smaller increase in the accuracy of the estimates for all correlations.

Fig. 6 shows the mean (a) and standard deviation (b) of the estimates of the capture zone width for various numbers of samples n and correlations r for both transmissivity distributions. Fig. 6 has been derived from cumulative distribution functions such as those in Figs. 4 and 5. Again, the organised case shows much larger biases than the random case (Fig. 6(a)). Auxiliary data are very efficient in reducing this bias.

In terms of the standard deviations of the capture zone widths (Fig. 6(b)), the two cases exhibit different behaviour. The standard deviation based on the organised transmissivity distribution is 410 m where no auxiliary data are used. With increasing correlation and number of auxiliary data, the standard deviation decreases substantially. For example, 70 additional samples of correlation 0.6 yield a standard deviation of 220 m. For the random case the improvement is much less pronounced. 70 additional samples of correlation 0.6 yield a standard deviation of 270 m.

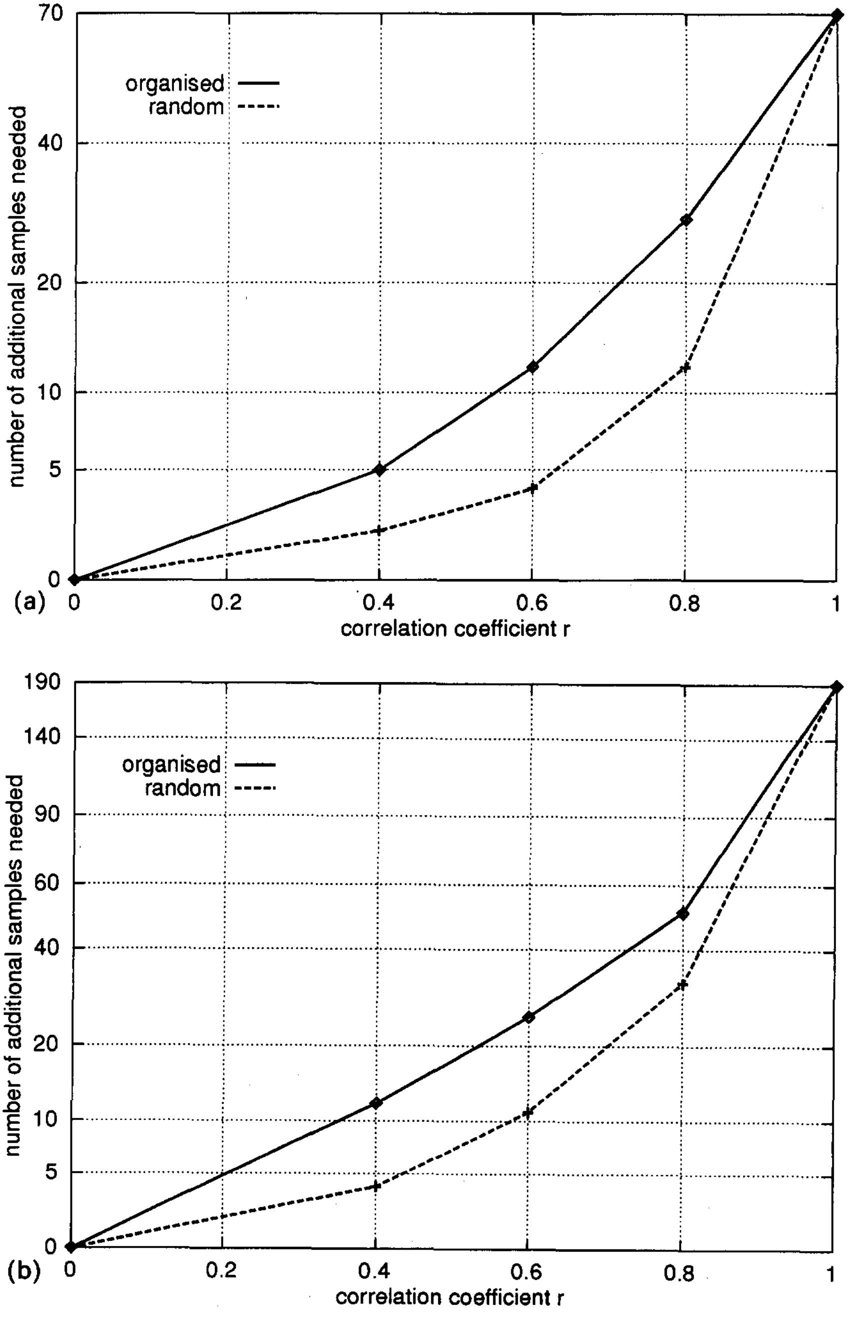


Fig. 7. Number of additional samples with perfect correlation (i.e. additional pumping tests) needed to obtain the same standard deviation of capture zone widths as (a) 70 or (b) 190 additional samples (i.e. geophysical data) with various correlations r.

4. Discussion

For the case of the organised transmissivity distribution, a substantial bias in the widths of the capture zone results from the use of 10 transmissivity values only. This is because the kriged patterns (without auxiliary information) are poor at portraying preferential flowpaths such as those included in this study (Fig. 1(a)). Clearly, kriging is based on the assumption that transmissivity is a random function that disregards the connectivity of extreme values. However, the inclusion of auxiliary data along with cokriging greatly enhances the ability to identify these patterns and to reduce the bias (Figs. 4 and 6(a)). This is true even for poorly correlated auxiliary data ($r = 0.4$). The case based on a correlated random field (Fig. 1(b)) exhibits almost no bias in the capture zone widths. This is because the assumptions that were used to create the realization of the random field (Fig. 1(b)) were similar to those on which kriging is based. This includes the assumption that the connectivity of extreme values is disregarded.

The standard deviation of the widths is a measure of the reliability or accuracy of the estimates. The standard deviation for the organised case with no auxiliary information is larger than for the random case (410 m as compared to 300 m) although the mean widths are identical (1060 m). In these cases (no auxiliary information) the scatter (i.e. standard deviation) is produced by the random location of the 10 transmissivities which are assumed to represent pumping tests. This indicates that in the organised case the selection of the location of the wells is much more important than for the random case. When auxiliary information is included, the reduction in standard deviation is much more pronounced in the organised case than in the random case (Fig. 6(b)). Clearly, the likelihood of identifying the buried stream channel is much larger with a large number of auxiliary data. Because there is no preferential flow in the random case, standard deviations are not reduced to the same degree.

The awareness that preferential flow may be important often guides the sampling strategy in practical field applications. The first step of characterising an aquifer system is often a geophysical survey. This gives rise to the question of the relative importance of pumping tests and auxiliary data. To this end, Fig. 6 has been redrawn to show more clearly the trade-off between the number of samples and correlation. Specifically, Fig. 7 shows the number of samples with perfect correlation ($r = 1$) needed to obtain the same standard deviation of capture zone widths as 70 (Fig. 7(a)) or 190 (Fig. 7(b)) additional samples with various correlations ($r < 1$). The samples with perfect correlation ($r = 1$) represent pumping tests. In other words, Fig. 7 indicates the number of pumping tests (and consequently boreholes) that can be saved by conducting a geophysical survey. For example, 12 pumping tests can be saved by a geophysical survey of 70 additional data points (Fig. 7(a)) correlated to transmissivity with $r = 0.6$ for the organised case examined here, while 25 pumping tests can be saved by a geophysical survey of 190 additional data points (Fig. 7(b)). As in Figs. 5 and 6, the results in Fig. 7 show that auxiliary information is particularly important when preferential flow is present. Typically, for a given number and correlation of auxiliary data, three times as many pumping tests can be saved in the organised case as compared with the random case.

The quantification of organisation and preferential flow paths will become more important in the future. The value of auxiliary data using cokriging has been examined here. There are other promising approaches that have potential for representing the connectivity of extreme values, such as methods based on the indicator technique (Journel, 1986; Kupfersberger, 1994). Much exciting work in this area can be expected.

5. Conclusions

Monte Carlo simulations are performed to assess the relative importance of the number of auxiliary data versus their correlation with transmissivities. The analyses are based on two hypothetical aquifers. The first involves a high transmissivity flowpath. The second is a realization of a correlated random field with the same spatial moments as the organised case. The accuracy of the estimated transmissivities is measured by cumulative distribution functions of the widths of the capture zone to a well. Results indicate that for the organised case the estimated widths in the case of including no auxiliary information are substantially biased. Auxiliary data are well suited to removing this bias by identifying preferential flowpaths. Auxiliary data also reduce the scatter (i.e. standard deviation) of the estimated widths significantly, which is a measure of the accuracy of the estimates. For the organised case, 70 samples of auxiliary data which are correlated to transmissivity by $r = 0.6$ outweigh the information from 12 additional pumping tests. For the case of the correlated random field, the benefit of using auxiliary data is much less pronounced both in terms of removing the bias and in terms of accuracy (i.e. standard deviation). It is concluded that auxiliary data are particularly useful for estimating transmissivity fields in the context of groundwater quality modelling when channelised flow is to be expected.

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