# Confidence and Uncertainty in Groundwater Contaminant Transport

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## 1. Introduction

Groundwater is an important, and often essential, water resource in many countries throughout the world particularly in arid and semi-arid regions. The storage capacity of large aquifers provides a capability for meeting short-term shortages induced by drought conditions. In addition, the overlying unsaturated soil provides a natural cleansing process through physical filtration, ion-exchange, biodegradation, plant uptake etc. which gives groundwater its (generally) good potable quality. However, pollution incidents can result in a release of contamination which is beyond the capacity of this natural buffering system. This will, in turn, result in a deterioration in groundwater quality which can place important resources at risk. In a world where there is increasing concern about the integrity of existing supplies under the constraints of potential climate change affecting recharge mechanisms, the increasing demand for water resources, and rising loadings of contaminants being released into the environment, the sustainability of groundwater is of increasing concern. Thus there is a need for tools to enable the environmental engineer to assess the likely risks of industrial, social and economic trends on the viability of groundwater resources. However, all this has to be undertaken within the context of the highly limited data which is generally available for groundwater studies. Hence, there is a need to be able to quantify this uncertainty in order to able to determine the level of confidence in groundwater model predictions. Such an approach also provides a more suitable framework for risk based assessments of groundwater contamination. This paper describes the problems associated with the heterogeneous properties of aquifers. It outlines the geostatistical methods increasingly being adopted to handle them and their impact on groundwater contaminant transport models. It highlights the need to incorporate uncertainty into models and illustrates this in connection with modelling well capture zones which are required to delineate groundwater protection zones.

## 2. Modelling Groundwater Flow

The equation which represents the flow of groundwater though porous rocks can be expressed as follows:

$$S\frac{\partial h}{\partial t} = \nabla \cdot K \nabla h + Q \tag{1}$$

where the potentiometric head $h(x,t)$ is the dependent variable, $Q$ is the groundwater flux due to recharge or pumping, and the storativity term $S(x)$ and hydraulic conductivity tensor $K(x)$ are coefficients which describe the aquifer's capacity to store and conduct water (Freeze and Cherry, 1979; de Marsily, 1986). Location and time are denoted by $\boldsymbol{x}$ and $t$ respectively. The potentiometric head represents the effects of gravitational potential energy and pressure forces:

$$h = \frac{p}{\rho g} + z \tag{2}$$

where $p(x,t)$ is the pore water pressure, $\rho$ is the fluid density, $g$ is the acceleration due to gravity, and $z(x)$ is the vertical elevation relative to a specified datum. Thus, given initial and boundary conditions for $h$ a unique solution can be obtained from **(1)**.

The groundwater specific flow rate $\boldsymbol{q}$ is given by Darcy's law:

$$\boldsymbol{q} = -K\nabla h \tag{3}$$

which allows the mean pore water fluid velocity $\boldsymbol{v}$ to be obtained as follows:

$$\boldsymbol{v} = \frac{\boldsymbol{q}}{n} \tag{4}$$

where $n(x)$ is the porosity of the porous medium from which the aquifer is comprised.

This equation has been widely used to characterise the movement of groundwater through aquifer systems. However, the flow field solution from this equation also provides the basis for representing the migration of contaminants dissolved in the groundwater through porous sub-surface media.

## 3. The Classical Contaminant Transport Equation

Traditionally the movement of contaminants through a groundwater flow field has been represented using the advection-dispersion equation (Bear & Bachmat, 1967; Fried & Combarnous, 1971). This assumes that the bulk of the contamination is transported at the same rate as the mean pore water velocity (assuming there are no interactions of the contaminant with the solid matrix of the aquifer). Superimposed on this is an assumed Fickian dispersion process, essentially similar to that of molecular diffusion only on a larger scale, which disperses the contamination around the mean position. This can be described as:

$$\frac{\partial(nc)}{\partial t} = \nabla\cdot\boldsymbol{D}\nabla c - \nabla\cdot(\boldsymbol{q}c) + Qc^{*} \tag{5}$$

where $\boldsymbol{D}(x)$ is the dispersion tensor and $Qc^{*}$ is the solute flux due to sources and sinks.

The classical dispersion theory has been developed by Taylor (1953), De Josselin De Jong (1958), Saffman (1959, 1960), Scheidegger (1960), Bear & Bachmat (1967), Fried and Combarnous (1971). This has demonstrated that the dispersion coefficient $\boldsymbol{D}$ is a function of the groundwater velocity and that the degree of dispersion differs in relation to the direction of the groundwater flow, i.e $D_L$ is the dispersion in the direction of groundwater flow and $D_T$ is the dispersion coefficient transverse to the flow direction. If the principal directions of dispersion are aligned with those for hydraulic conductivity then the dispersion tensor is limited to its three principal components, hence:

$$\boldsymbol{D} = \begin{vmatrix} D_L & 0 & 0 \\ 0 & D_T & 0 \\ 0 & 0 & D_T \end{vmatrix} \tag{6}$$

where $D_L = \tau D^{*} + a_L|\boldsymbol{v}|$ and $D_T = \tau D^{*} + a_T|\boldsymbol{v}|$ and $a_L$ and $a_T$ are the longitudinal and transverse dispersivities of the porous medium respectively. Theoretically these parameters are fundamental properties of the medium. However, Gelhar et al. (1992) have shown that applications of the above model to contaminant transport behaviour has demonstrated a scale-dependent behaviour in aquifer dispersivity (Figure 1).

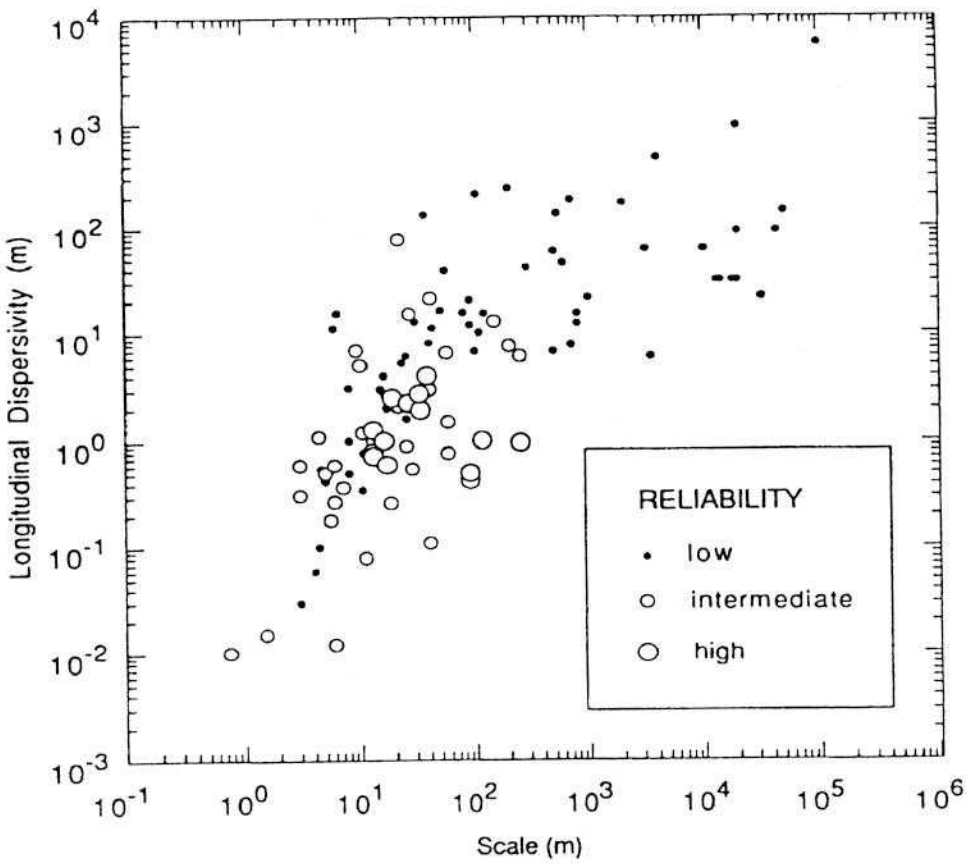


Figure 1. Field longitudinal dispersivity data classified according to reliability (from Gelhar et al., 1992)

## 4. Scale dependent aquifer properties

The underlying cause of this variation in dispersivity lies in the processes which govern the formation and subsequent changes in the structure of the porous medium (e.g the fluvial geomorphology which effects the structure of alluvial aquifers). These processes operate over a wide range of scales. Their greatest hydrogeological influence is on the hydraulic conductivity parameter *K*. An example of the degree of variability which can occur is shown in figure 2. This shows detailed hydraulic conductivity analyses of the Borden aquifer in Canada (Sudicky, 1986). The ranges in hydraulic conductivity measured over a distance of a few metres shows ranges of about two orders of magnitude. Clearly such variation creates problems. Traditionally this has been approached through the determination of effective parameters at a particular spatial measurement scale (e.g. centimetres for permeameter tests, metres for piezometer tests, hundreds of metres for pumping tests, kilometres if inverse model calibration undertaken). However, whilst these effective parameters are generally sufficient for head field simulations, they tend to introduce bias when contaminant transport simulations are conducted. This is because the detailed variations in hydraulic conductivity, in turn, result in small-scale variations in groundwater flow and cause mechanical dispersion of contamination. Hence, in order to capture these effects the detailed structure of the hydraulic conductivity field is required. This, however, is impossible to do on a deterministic scale. The amount of disruption to the aquifer would distort its behaviour notwithstanding the costs involved. An alternate method, therefore, is to use geostatistics to capture the general spatial characteristics of the hydraulic conductivity field (Gelhar, 1993).

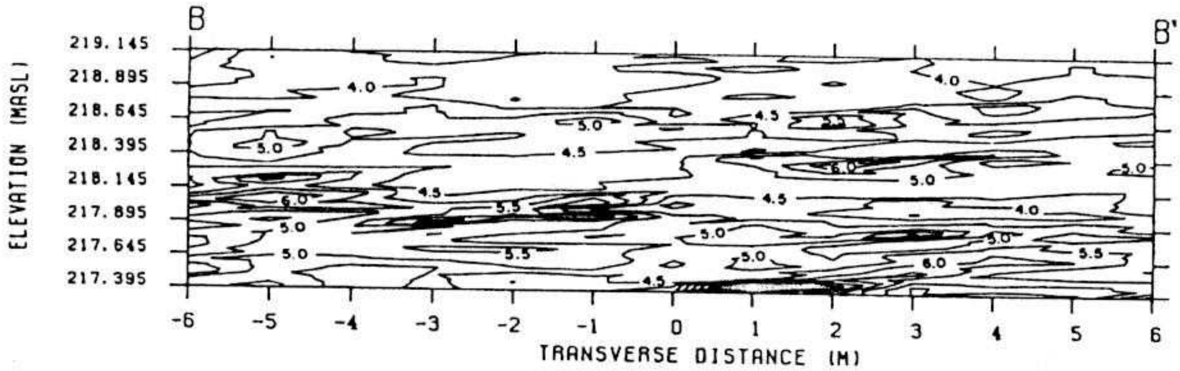


Figure 2. Distribution of $-\ln(K)$ along a vertical cross-section (contour interval = 0.5; vertical scale exaggerated; $K < 10^{-3}$ cm/s in stippled zone) (Sudicky, 1986)

Realisations of an aquifer's hydraulic conductivity field can instead be generated from a statistical analysis conditioned on to points where observed information is available. This is achieved through the construction of a semi-variogram (Figure 3) which describes the spatial correlation structure of hydraulic conductivity for the aquifer. Figure 4 shows a near-surface alluvial aquifer which underlies a sloping topographic field. The hydraulic conductivity field has been generated using a relatively low variance, spatially correlated hydraulic conductivity field with horizontal and vertical correlation lengths of 2.5 and 0.5 grid elements respectively (Tompkins et al., 1994). The random field was generated using the Turning Bands Method (Tompson et al., 1989) using 98 radial line projections uniformly spaced in three dimensions. This was used to create a field comprising 100x100x20 grid elements, (a total of $2\times10^5$). In order to visualise its structure an arbitrary threshold value was used to highlight low hydraulic conductivity regions (Butler et al., 1997). The spatial structure of the field can be seen by the shapes of these zones. They represent locations where groundwater flow will be lower than the surrounding space. Therefore contaminant particles introduced into the simulated groundwater flow field will tend to move preferentially along zones of high hydraulic conductivities. However, any contaminants which happen to enter the low conductivity regions will tend to become trapped as a result of the low flow velocities.

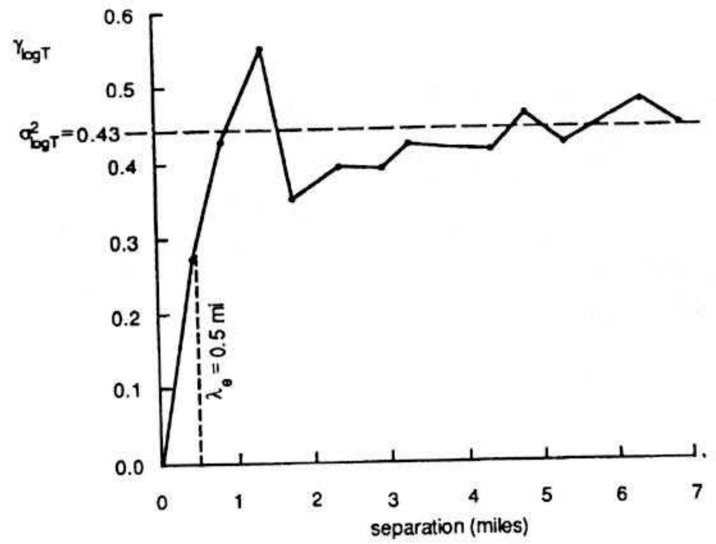


Figure 3. Estimated semi-variogram of log transmissivity for the Cortaro aquifer (Gelhar, 1993).

## 5. Lagragian contaminant transport simulations

Incorporating these spatial variations in hydraulic conductivity into a groundwater flow model enables spatially correlated variations in the groundwater flow field to be generated. If the resolution of the flow field can be made fine enough then the movement of contaminants through the aquifer can be simulated by tracing the pathways of conservative (i.e. non reactive) particles placed in the simulated groundwater flow field. This represents a Lagragian view of contaminant transport rather than the more traditional Eulerian approach. Thus the $i^{th}$ particle's displacement vector $\boldsymbol{x}_i(\mathrm{t})$ at time $t$ is the integration of the mean pore water velocity $\boldsymbol{v}$:

$$\boldsymbol{x}_i(t) = \int^{t} \boldsymbol{v}.dt = \int^{t} \frac{\boldsymbol{q}}{n}.dt \tag{7}$$

Hence, the migration of a plume of contamination through an aquifer can be reproduced by the introduction of a cloud of particles and the tracking of their subsequent movement in time. It is evident, however, that in order to reproduce the types of variation observed in the field the model simulation needs to employ an extremely detailed grid mesh. Figure 5 shows an example of a 'plume' of particles from a surface contamination site migrating towards a well.

The simulation shows the site to be located somewhere within the capture zone of the well and thus able to contaminate the water supply. Therefore, if a protection strategy for the well is to be developed an area denoting similar locations around the well needs to be identified. This can be readily obtained by introducing particles over the simulated flow field and observing which end up at the well. The particle capture zone obtained from the model simulation is shown superimposed on the top of the aquifer in Figure 6. This allows a protection zone for the well to be marked on the ground. Armed with this information a regulating authority would be able to provide advice and guidance on whether planning permission should be granted for proposed developments which might have a groundwater contamination risk and therefore threaten the integrity of the groundwater source.

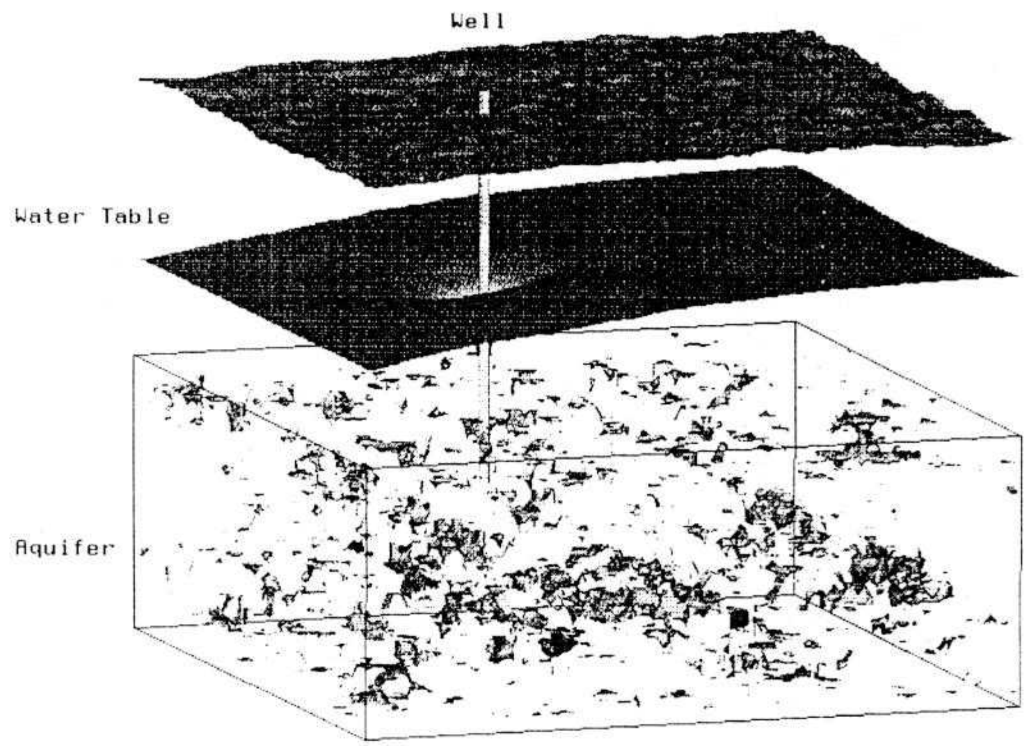


Figure 4. Visualisation of a spatially correlated unconfined aquifer with uniform recharge and a well abstraction.

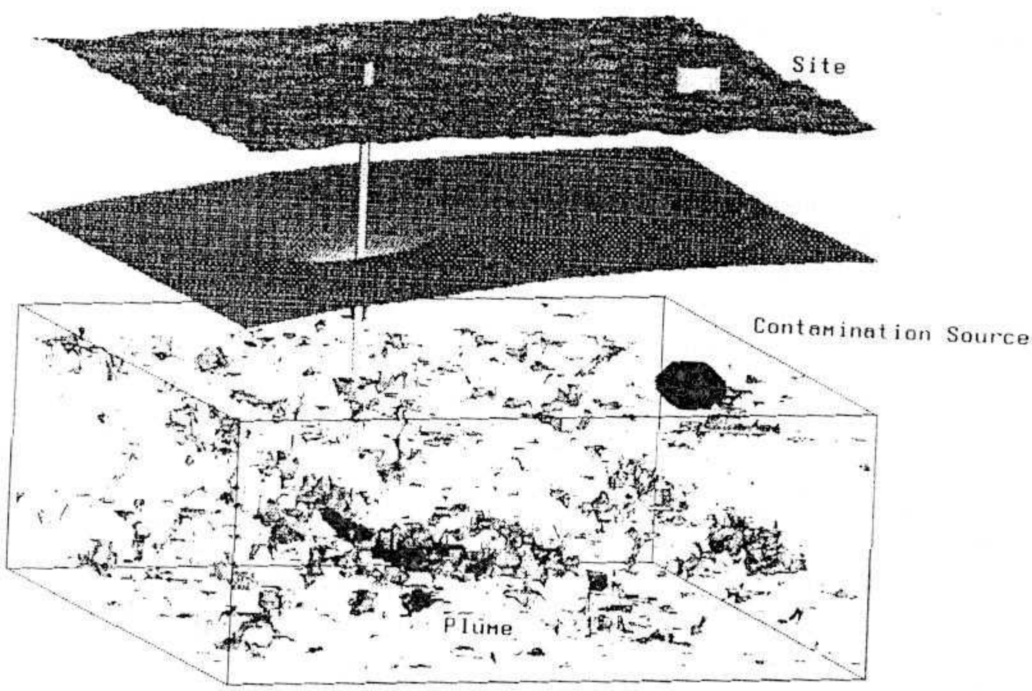


Figure 5. Migration of contaminant plume from source towards supply well

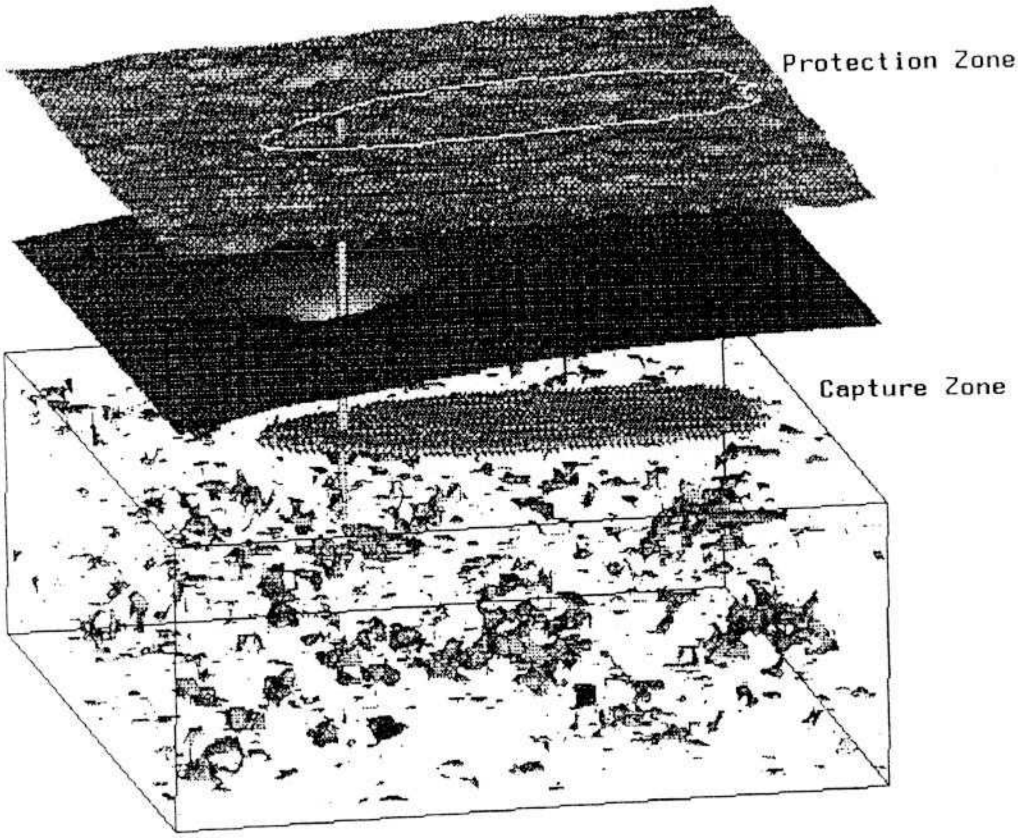


Figure 6. Definition of Well Capture Zone delineating source protection zone.

## 6. Stochastic contaminant transport simulations

The approach described in the previous section involved generating a highly detailed hydraulic conductivity field. However, this is only one realisation of what is actually true. This is because knowledge of the exact structure of the aquifer is extremely poor due to the limited information being available from a small number of sampling points (i.e. boreholes). Hence, there is a high degree of uncertainty in the representation and simulation of the aquifer. However, the methodology provides a means of practically incorporating this uncertainty into the model simulations and quantifying it. The above hydraulic conductivity field can be regarded as one realisation of the true field and hence the resulting protection zone as one realisation of the 'true' capture zone. By undertaking a series of stochastic simulations using the same underlying statistical properties an ensemble of capture zones can be generated. Therefore the 'capture zone' could instead be represented as a spatial probability distribution. Thus the uncertainty as to whether a point lies within the true capture zone can be estimated. Such an approach is shown in Figure 7. Thus planning and protection considerations can be implemented according to the level of probability that a particular location lies within a capture zone combined with the associated risk of the site polluting the aquifer. This, therefore, represents a more reasonable solution for protecting groundwater supplies and ensuring sustainable future resources.

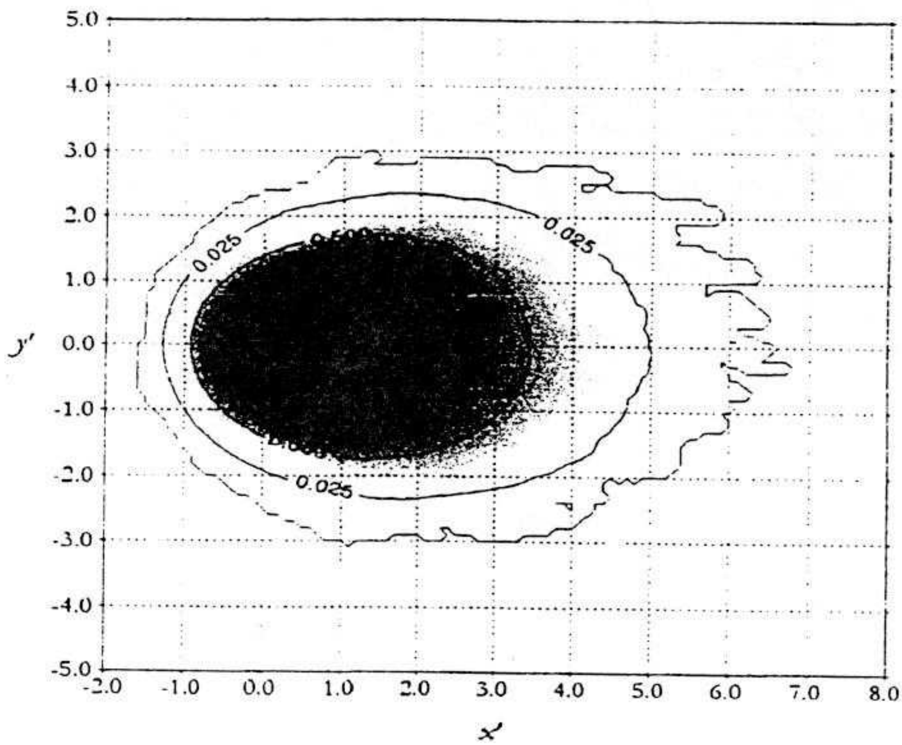


Figure 7. Contour plot of capture zone probability distribution for an abstraction well in a spatial correlated hydraulic conductivity field (van Leeuwen, 1997).

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