WELL CATCHMENTS ESTIMATION IN HETEROGENEOUS AQUIFERS WITH A STRATIFIED MODEL

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ABSTRACT

In natural formations the porous media heterogeneity influences the capture zone delimitation and considerable differences can result from the homogenous case. In the last decade several approaches were proposed to solve the problem, but generally they necessitate of the improbable knowledge of the aquifer's statistical properties. In the note a method is proposed to delimitate wellhead protection areas in a bounded artesian aquifer where hydraulic conductivity is assumed as a spatially homogeneous random function. To give a probabilistic estimation of well catchments, we suggest that the 3-D aquifer can be suitably represented by a perfectly stratified model that is defined by the use of three parameters only: the expected value and the variance of the hydraulic log-conductivity, and the constant thickness of aquifer's layers. While the log-conductivity expected value is derived from a standard pumping test, to define the variance and a proper number of layers, a multilevel tracer test has to be developed. To validate the proposed method pumping and tracer tests were developed in a fully 3-D synthetic aquifer and experimental results are processed to define the stratified model's parameters. Isotropic and anisotropic conditions characterized by low and moderate hydraulic log-conductivity variance are investigated. In all cases the well catchment and time-related capture zones obtained by the suggested approach fit quite well the corresponding areas that can be recognized in the synthetic aquifer.

1. INTRODUCTION

Field investigations and theoretical analyses on well capture zones play an important role in aquifer protection and in the design of remediation systems for groundwater's pollution. In this case the heterogeneity of natural formations plays a relevant role mainly related to the spatial variability of hydraulic conductivity. So that the time-dependent capture zone drawn for an homogeneous porous medium with an uniform background hydraulic gradient [Bear and Jacobs, 1965] can substantially differ from evidences encountered in real field cases. Starting from the work by Varljen and Shafer [1991], where the conditioning effect on the catchment's area design was examined, many studies have been developed during the last decade by taking into account a random variability of hydraulic conductivity. By use of Monte Carlo simulations Franzetti and Guadagnini [1996] and Guadagnini and Franzetti [1999] analyze the influence of transmissivity variance and develop an empirical relationship to define the capture zone in 2-D unbounded domains. In van Leeuwen et al. [1998, 2000] the combined effect of hydraulic transmissivity variance and spatial correlation were considered in both fully confined and leaky-confined aquifer by use of conditional and unconditional Monte Carlo simulations. Different approaches incorporating first-order second-moment approximation were pursued by Kunstmann and Kinzelbach [2000], Stauffer et al. [2002] and Bakr and Butler [2005], while in Lu and Zhang [2003] a moment approach is followed to obtain probabilistic time-related capture zones.

All the cited works were developed under the hypothesis that the transport process is dominated by the spatial variability of the hydraulic transmissivity, that is the depth-averaged aquifer property whose integral scale – of order of 10^2-10^3 m [Dagan, 1986] – is comparable with the common size of well head protection areas. Moreover the transmissivity distribution is assumed as known and this is not the usual situation in real word cases. Although a fully 3-D analysis seems to be more appropriate to describe the transport phenomenon in a heterogeneous media surrounding a well, the complexity of this kind of model and the generalized lack of proper input data suggests to switch to a simplified model.

Theoretical considerations and numerical results suggest that the capture zone definition is mainly related to vertical variations of hydraulic conductivity [Savini and Salandin, 2002]. Following this way, in the present work we assume that the transport process that takes place near a pumping well in a natural aquifer can be suitably represented by a perfect layering model, where the hydraulic conductivity K varies along the vertical coordinate only. The random K is constant in each layer, and its correlation length is proportional to the layer thickness along the vertical direction, while in the horizontal plane it becomes infinity. So that the spatial variability of hydraulic conductivity, assumed as usual log-normally distributed, is completely defined by the knowledge of the following quantities: thickness of layers (or number of layers in the total aquifer depth), mean and variance of hydraulic log-K. To assess these parameters by in situ developed pumping and tracer tests and to define time-related capture zones via the stratified model, a new technique is here proposed.

The paper is organized as follows. In Section 2 a brief description of the stratified model schematization is given, while the 3-D synthetic aquifer, as well as the development and interpretation of pumping and tracer tests, are illustrated in Section 3. Results of numerical simulations are discussed in Section 4 and a collection of main conclusions closes the note.

2. THE LAYERED MODEL SCHEMATIZATION

Let's consider a 3-D confined aquifer affected by an uniform gradient $\mathbf{J} = (J,0,0)$ where a fully penetrating well is pumping the constant discharge Q. The aquifer total thickness is B, with planimetric longitudinal (in the direction of the gradient) extension L and transversal width A (Figure 1). Assumed the origin of the coordinate system in the middle of lower left corner with x_3 in the upward direction, planimetric coordinates of well are x_1=s and x_2=0.

The travel time τ employed by a conservative solute parcel starting at $\mathbf{x}$=$\mathbf{b}$ and time t=t_o to reach the well located at $\mathbf{x}_w$=$(s,0,x_3)$ can be obtained from

$$\tau = \int_{\mathbf{b}}^{\mathbf{x}_w} d\mathbf{X}/\mathbf{v}(\mathbf{X}) \qquad (1)$$

where $\mathbf{v}$=$\mathbf{q}/n$ is the Lagrangian velocity of the particle travelling along the trajectory of equation $\mathbf{x}$=$\mathbf{X}(t;\ \mathbf{b},\ t_o)$ and n is the effective porosity assumed spatially constant. Due to the spatial variability of K, the travel time is, according to the Darcian velocity $\mathbf{q}=-K\cdot\nabla\Phi$, a random variable too.

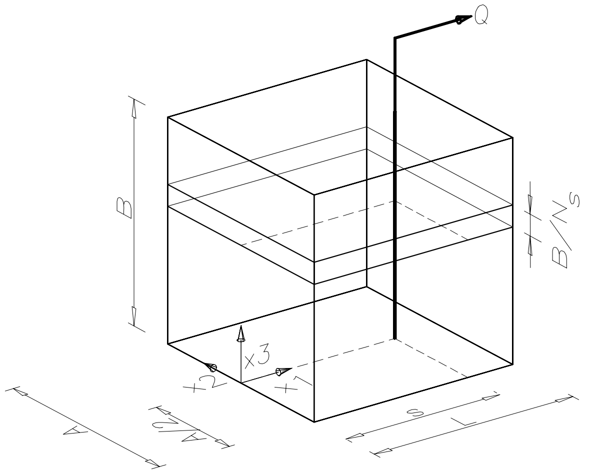

FIGURE 1. Sketch of the 3-D domain.

In the stratified model the total thickness B is subdivided in a number N_s of equally spaced layers each of those characterized by a constant random hydraulic conductivity K_k. The fraction ΔQ_k that flows to the well along each layer is

$$\Delta Q_k = Q \cdot K_k \,/\, \textstyle\sum_1^{N_s} K_i \;, \tag{2}$$

so that the 3-D domain reduces to a collection of N_s independent layers where the flow and transport are strictly 2-D and computations can be developed separately.

For the unbounded domain a closed form solution of (2) is given by Bear and Jacobs [1965], while in the finite aquifer the same result can be obtained via a semi-analytical procedure. Assumed the following prescribed potential head conditions: $\Phi=\Phi_1$ at $x_1 = 0$, $\Phi=\Phi_2$ at $x_1 = L$ and no-flux at the remaining boundaries, by use of the principle of superposition and conformal mapping in the complex plane [Muskat, 1937], the spatial distribution of Φ results

$$\Phi(x_1,x_2) = \Phi_1 - \frac{\Phi_2-\Phi_1}{L}x_1 + \frac{\Delta Q_k}{4\pi KB}\sum_{j=-\infty}^{+\infty} \ln \frac{\cosh\left(\frac{\pi x_2}{L} - \frac{j\pi A}{L}\right) - \cos\left(\frac{\pi x_1}{L} - \frac{\pi s}{L}\right)}{\cosh\left(\frac{\pi x_2}{L} - \frac{j\pi A}{L}\right) - \cos\left(\frac{\pi x_1}{L} + \frac{\pi s}{L}\right)}, \tag{3}$$

and the travel time (1) is deduced by numerical quadrature of velocities achieved from (3) by differentiation.

We consider a tracer instantaneous injection along the vertical axis $\mathbf{x}=(b_1,b_2)$ where the solute can be described as the ensemble of a finite number of particles each of mass m_i. For the generic k-th layer the mean travel time and variance to reach the well are defined as

$$\bar{\tau}_k = \sum_{i=1}^{Np,k} m_{i,k}\tau_{i,k} \Big/ \sum_{i=1}^{Np,k} m_{i,k} \quad \text{and} \quad s_{\tau,k}^2 = \sum_{i=1}^{Np,k} m_{i,k}\left(\tau_{i,k}-\bar{\tau}_k\right)^2 \Big/ \sum_{i=1}^{Np,k} m_{i,k} \;, \tag{4}$$

where $\tau_{i,k}$ is the travel time for the *i-th* particle captured by the well in the *k-th* layer and $N_{p,k}$ is the total number of these particles. Note that in a real 3-D heterogeneous domain, due to the vertical displacement, collected particles that contribute to (4), are not necessarily originating in the same *k-th* layer, while in the stratified schematization is always $s_{\tau,k}^2=0$.

With reference to the entire thickness B of the aquifer, the mean travel time m_τ and the uncertainty R_τ^2 around its value can be computed by use of the first of (4). Defined as $m_k=\sum m_{i,k}$ the total mass of solute captured in the *k-th* layer, one obtains

$$m_\tau = \sum_{k=1}^{Ns} m_k \bar{\tau}_k \Big/ \sum_{k=1}^{Ns} m_k \quad \text{and} \quad R_\tau^2 = \sum_{k=1}^{Ns} m_k \left(\bar{\tau}_k - m_\tau\right)^2 \Big/ \sum_{k=1}^{Ns} m_k \ . \tag{5}$$

The uncertainty given by the second of (5) mainly depends on the number of layers N_S, while it doesn't affect the travel time variance that can be computed by

$$s_\tau^2 = \sum_{k=1}^{Ns} \sum_{i=1}^{Np,k} m_{i,k} \left(\tau_{i,k} - m_\tau\right)^2 \Big/ \sum_{k=1}^{Ns} \sum_{i=1}^{Np,k} m_{i,k} \ . \tag{6}$$

If the real aquifer is well accomplished by the stratified model the R_τ^2 value approaches the s_τ^2 one, whereas the latter condition doesn't imply that transport in a 3-D heterogeneous media can be described by a simply layered model. This is mainly due to the fact that in the real word $s_{\tau,k}^2$ is always different from zero, reflecting the erratic path followed by single parcel of solute due to the spatial variability of hydraulic conductivity and to the pore scale dispersion. By the stratified model only the quantities that contribute to the relationships (5) are considered as a function of the layers number and the mean and the variance of hydraulic log-conductivity. Nevertheless this rough schematization can be useful to assess the capture zone uncertainty near the well, where the transport process seems to be dominated by vertical variations of hydraulic log-conductivity [Savini and Salandin, 2002].

3. IDENTIFICATION OF MODEL PARAMETERS

3.1 The synthetic aquifer

Identification of the layered model parameters requires the development and the proper interpretation of pumping and tracer tests in a real aquifer. To simply achieve several results and to test the performance of theoretical developments described in Section 2, we realize a synthetic 3-D aquifer of size L=48 m, A=40 m and B=20 m with the following imposed boundary conditions: constant piezometric head Φ_1=100.48 m at x_1=0 and Φ_2=100.00 m at x_1=48.00 m, and no-flux on the remaining sides, being J=0.01 the mean gradient along x_1. A vertical fully penetrating pumping well of 0.25 m of diameter is located at the abscissa s=34 m while the position of the piezometer/injection well was set at x_1=26 m aligned in the mean flux direction. The spatially random hydraulic conductivity $K(\mathbf{x})$ is assumed log-normally distributed (Y=ln$K$) with expected value $\langle Y \rangle$, variance σ_Y^2, and exponential correlation structure $\rho_Y(\mathbf{d})=\exp\{-[(x_1^2+x_2^2)/e^2+x_3^2]^{1/2}/\lambda_v\}$ where **d** is the oriented separation vector. Defined as λ_o and λ_v the horizontal and the vertical correlation lengths respectively, $e=\lambda_o/\lambda_v$ is the anisotropy ratio. The vertical correlation length was set as always λ_v=1 m, while two different conditions of anisotropy e=1 and e=8 were considered. The aquifer was discretized into a regular grid of 2,457,600 cubic elements of constant lateral size of 0.25 m. The 3-D correlated hydraulic conductivity field was computed by use of an algorithm that generates real random data on the regular grid by performing an inverse Fourier transform on the spectral representation of the variables [*Robin et al.,* 1993]. Two different imposed hydraulic log-conductivity variance values σ_Y^2=0.1 and 0.5 were considered, while the expected value was set always <Y>=−6.556. In the synthetic aquifer is assumed that the dispersion was dominated by heterogeneity of K and process related to the pore scale are disregarded.

3.2 Pumping and traces tests interpretation

To achieve drawdown suitable results in our limited domain, we set the ratio between elastic storage and hydraulic conductivity geometric mean S_S/K_G=9.50 s/m^2, and pumping discharge Q=20 l/s. The pumping test was simulated by integration on the 3-D domain of

$$\nabla\left(K\,\nabla\Phi\right)+Q'=S_S\,\frac{\partial\Phi}{\partial t}. \tag{7}$$

with proper initial and boundary conditions and were Q' is the well discharge for unit of volume. The resulting data was analyzed by use of the well known Theis relationship.

The tracer tests were developed in steady state, with Q=8 l/s, and by considering an instantaneous injection of passive solute along the entire thickness of the aquifer in the well located at x_1=26 m. The tracer evolution was simulated by following trajectories of about 2000 particles uniformly distributed. In both time dependent and steady state cases, the computations were performed by use a finite volume (FV) technique coupled with a Pollock velocity post processor that gives a good compromise between the solution accuracy and the requirements in term of memory amount and CPU time [Salandin et al., 2000].

We assume that the travel times are measured by use of a multilevel sample equipment located in the pumping well to achieve depth-differentiated multilevel breakthrough curves [Ptack et al., 2004] with a spatial resolution of about 0.80 m. From the tracer test, 24 breakthrough curves are measured in the synthetic aquifer and, by use of the first of (4), up to 24 mean travel times m_k were computed. The same scattered data of all breakthrough curves were rearranged in a different way, by computing mean travel time on sample of 2, 3, 4, …, 24 adjacent sampling levels. This leads different evaluations of m_k and R_τ^2 as a function of the different number of layers assumed in the application of relationships (4) and (5).

In Figure 2 the results for different combinations of anisotropy (e=1 and 8) and log-conductivity variance (σ_τ^2=0.1 and 0.5) are interpolated by the exponential relationship

$$R_\tau^2=s_\tau^2(1-e^{-\beta\cdot Ns}), \tag{8}$$

were the only parameter β is deduced by a best fitting of different values of R_τ^2 obtained from measured data by varying the number of layers in the application of (4).

The choice of the asymptotic interpolating relationship (8) can be justified as follows. As we increase the number of layers, the value of R_τ^2 will reach certainly a sill if: *i*) the real aquifer heterogeneity is mainly dominated by horizontal stratifications; *ii*) their thickness is greater than the value B/N_S adopted in the layered model.

Clearly in a real aquifer the dispersion/uncertainty is related to the spatial moments of the 3-D erratic path of trajectories. In a layered schematization, where the (discrete) vertical variation only of hydraulic conductivity is taken into account, these effects can be taken into account by a proper choice of the σ_Y^2 variance and of the finite number of layers N_S only.

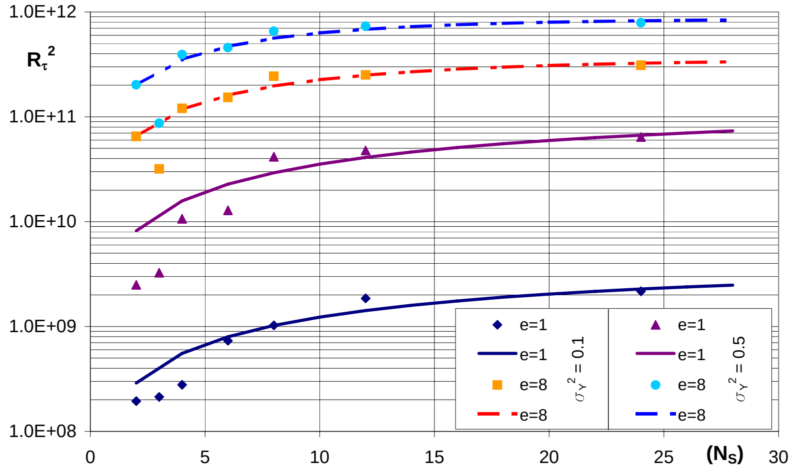

FIGURE 2. Dependence of travel time variance upon number of layers N_S.

So that the number of layers N_S was chosen as the value that realizes for the specific interpolating curve of Figure 2 the value R_τ^2=0.95s_τ^2. From these N_S values and <*Y*> deduced via Theis' analysis of drawdown, the application of (1) and of (5) on the tracer test data leads the σ_Y^2 estimated parameters that owing to the layered model.

In Table 1 the N_S and σ_Y^2 parameters deduced from tracer tests and the <*Y*> obtained via the drawdown analysis, are collected and compared with the real-field generated properties. Marked differences between the σ_Y^2 generated and estimated values are manifest and this fact confirms that the perfect layering is a rough schematization of a real aquifer and it is unable to identify a real heterogeneity behaviour. Nevertheless we will demonstrate in the next Section as it can be suitably adopted to give a measure of probabilistic time-related capture zones.

TABLE 1. Results for interpretation of four different domain type.

case	aquifer generated properties		model estimated parameters		
$e=\lambda_o/\lambda_v$; σ_Y^2	<Y>	σ_Y^2	<Y>	Ns	σ_Y^2
1; 0.1	-6.550	0.0909	-6.5459	71	0.0383
1; 0.5	-6.544	0.4544	-6.5403	51	0.0989
8; 0.1	-6.557	0.0867	-6.5120	120	0.1282
8; 0.5	-6.558	0.4334	-6.4229	52	0.3237

4. TIME-RELATED CAPTURE ZONE: RESULTS AND DISCUSSION

By use of the layered model described in Section 2 in conjunction with parameters of Table 1 we carry out a probabilistic travel time analysis via a Monte Carlo approach. At each iteration a set of N_S conductivity values log-normally distributed with estimated mean <*Y*> and variance σ_Y^2 was generated and the flow field in each layer was deduced by use of (3), being the continuity across layers expressed by (2). Travel times to reach the well are obtained by numerical integration in each node of a plane regular grid spaced of 0.50 m. The use of relationship (3) ensures the perfect agreement between the boundary conditions of the 3-D aquifer and the stratified model. The latter can be defined by use of isoprobable isochrones $m_\tau(P)$, where P is the probability that a particle reaches the pumping well in a shorter time than a prescribed value. As an example, $m_\tau(0.50)$=200, defines univocally the time-related capture zone where the released particles have a probability of 50% to reach the well in a time less than 200 hours. This is done by sorting in each grid node after N_{MC} simulations the array of travel times of dimension $N_C=P_C \cdot N_{MC} \cdot N_S$, where P_C is the capture percentage. So that it is univocally defined the time corresponding to the specific percentile t_{50} and from the ensemble of all nodal values we can draw the isochrones $m_\tau(0.50)$. In the Figures from 3 to 6 the time-related capture zone obtained by the layered model (hatched line) are compared with depth-averaged evidences deduced from the synthetic 3-D aquifer (continuous line) in all the cases (e=1 and 8, σ_τ^2=0.1 and 0.5) here considered. The results refer to the $m_\tau(P)$=200 hours with probability of 10%, 50% and 90%, corresponding to the percentiles t_{10}, t_{50}, and t_{90} respectively. From the comparison it is clear as the model quite well accomplishes isochrones referring to both the median percentile t_{50} and the deviates t_{10} and t_{90} also.

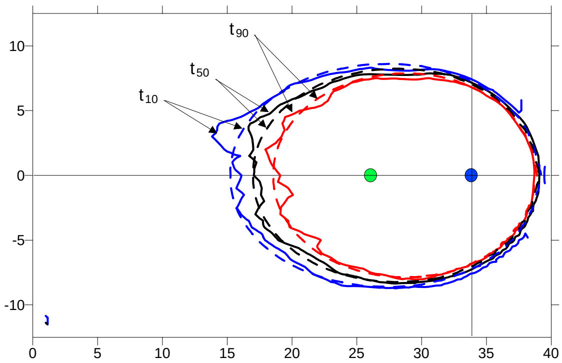

FIGURE 3. Percentiles t_{10}, t_{50} and t_{90} for 200 hours isochrones in aquifer with e = 1 and σ_Y^2 = 0.1. NMC = 200.

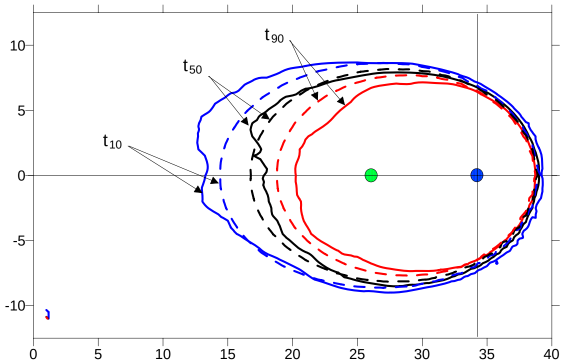

FIGURE 4. Percentiles t_{10}, t_{50} and t_{90} for 200 hours isochrones in aquifer with e = 8 and σ_Y^2 = 0.1. NMC = 200.

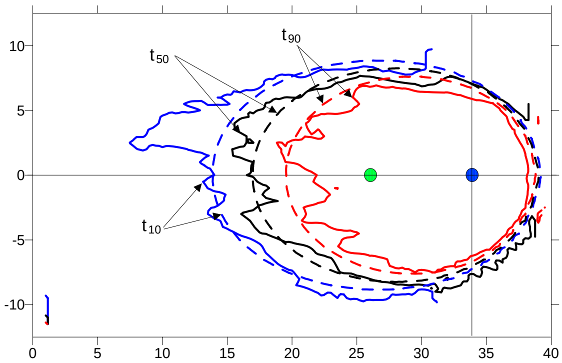

FIGURE 5. Percentiles t_{10}, t_{50} and t_{90} for 200 hours isochrones in aquifer with e = 1 and σ_Y^2 = 0.5. NMC = 1000.

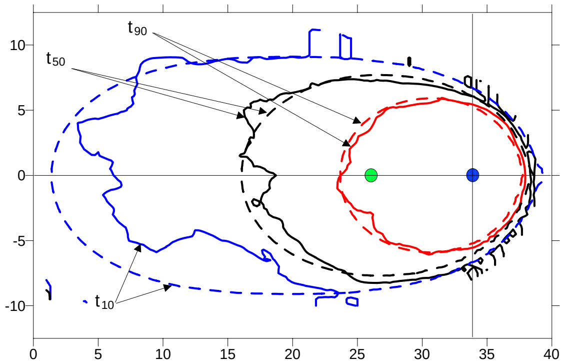

FIGURE 6. Percentiles t_{10}, t_{50} and t_{90} for 200 hours isochrones in aquifer with e = 8 and σ_Y^2 = 0.5. NMC = 1000.

5. CONCLUSIONS

By use of a layered model, in the paper a new technique useful to define the time-related capture area near a well drilled in naturally heterogeneous aquifers is suggested. From the results of numerical simulations here reported the following main conclusion can be drawn.

1. The perfectly layered model gives a rough description of the 3-D random hydraulic conductivity spatial variation taking place in natural formations. Nevertheless by this model we can accomplish the statistics of transport near a pumping well, where the phenomenon seems to be dominated by the vertical variability of *K*.

2. Several numerical experiments were performed by taking into account two values of log-conductivity variance (σ_τ^2=0.1 and 0.5) and two anisotropy ratios (*e*=1 and 8). In each case we infer the layered model parameters from pumping and multilevel sampling tracer tests developed on a 3-D synthetic aquifer simulating the reality.

3. Although estimated log-conductivity variance differs from synthetic aquifer data, probabilistic time-related capture areas deduced by simplified model fits quite well field cases. The median isochrone resulting from depth-average of 3-D data is always well accomplished, while extreme percentiles (10% and 90%) isochrones denote some differences from the model prevision that seem to be enhanced in the anisotropy case.

4. These differences can be attributed to the distance between injection and pumping well that for *e*=8 is comparable with the horizontal correlation length of 3-D aquifer, so that this fact affects the uncertainty estimation from tracer test analysis.

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