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Delineation of capture zones by an integrated surface/subsurface model using the GLUE methodology

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Abstract A synthetic reference capture zone was generated using stochastic distributed hydraulic conductivities. The corresponding conceptual model incorporated errors in the geological model through a rough zonation of the hydraulic conductivities. The geological model, precipitation and hydraulic conductivities were estimated using the Generalized Likelihood Uncertainty Estimations methodology (GLUE), where Monte Carlo simulations are performed and the model results are conditioned on head and river discharge. The estimated capture zones were presented as likelihood maps and the 99% prediction zone covered the reference capture zone. As the degree of heterogeneity increased, the 99% prediction zone failed to cover the reference capture zone.

Key words capture zone; GLUE; integrated model; model error; stochastic simulation; uncertainty

INTRODUCTION

The size and location of capture zones are very important outputs from groundwater models. Regulations on land use and responses to point pollution are often implemented on the basis of capture zone estimates. These estimates can be made in a number of ways, using methods ranging from simple analytic solutions to sophisticated numerical models such as MIKE SHE (Abbott *et al.*, 1986) or MODFLOW (McDonald & Harbaugh, 1988), including three-dimensional (3-D) transient flow.

Regardless of whether an analytic solution or a numerical model is used for the estimate, capture zone modelling is fraught with potential error. Analytic solutions require more or less ideal aquifers, while numerical models are capable of dealing with highly non-ideal problems. In principle it would be possible to set up a numerical model that would produce an error free capture zone, provided the data basis was complete. In practice, however, this is never the case.

The question therefore is: to what extent does an incomplete data basis influence the numerical estimation of capture zones? In order to answer this, we need to uncover the unknown or uncertain parameters involved. Capture zones are derived from groundwater pore velocities, and these in turn originate from the governing equations relating to groundwater flow. Thus any uncertainty in the estimation of capture zones must originate from inadequate governing equations, from uncertainty in the parameters involved in these equations (hydrogeological parameters and sink/source terms), from incorrect boundary conditions or from the numerical solution method used.

The present study is confined to the treatment of uncertainty in the hydrogeological parameters and in the sink/source terms.

The spatial variability of the hydrogeological parameters within a geological unit is often not recognizable from the available geological surveys. It is therefore often difficult to identify any heterogeneity within such a unit, and consequently rough zonations of the parameters must be used. However, point measurements of, e.g. hydraulic conductivity, and large head variations over short distances, indicate the existence of considerable heterogeneities.

The present study concerns the estimation of the size and location of capture zones in a synthetic groundwater catchment. Work on synthetic set-ups is considered an important step towards applying methods for estimating capture zones and their uncertainty to real studies. Synthetic set-ups provide an obvious opportunity to validate the methods used in estimating capture zones.

The objectives of this study are:

- To examine the effect of errors in the conceptual model on the prediction of capture zones.
- To evaluate the GLUE methodology for propagating model errors through the numerical model to the capture zone estimate.

THEORETICAL BACKGROUND

Governing equations

The groundwater flow was described by the 3-D heat equation (Freeze, 1979), and the river and overland flow was described by a 2-D diffusive wave approximation of the Saint Venant equations (Liggett, 1975).

The GLUE methodology

The traditional calibration approach aims to find a unique set of parameters that produces an optimal simulation of the behaviour of a given study area.

Beven & Binley (1992) argue against the existence of a unique optimal parameter set, proposing instead the concept of equifinality of model structures and model parameters. According to this concept, a number of models and parameters may be accepted as equal or near equal simulators of the system.

A fundamental step in the GLUE methodology is the calculation of a likelihood measure for every realization. The likelihood measure is calculated on the basis of the residuals between observed and simulated data. It represents a subjective measure of model performance given a parameter realization. A number of likelihood measures have been suggested in the literature (e.g. Beven & Binley, 1992; Beven & Freer, 2001; Feyen *et al.*, 2001). In the present study the calculation of the likelihood measure was divided into two steps: the first step was to calculate a likelihood measure for every single observation point, L_i; the second was to combine these individual likelihood measures into a global likelihood measure for the given realization, L_g.

Observation point likelihood measure

The observation point likelihood measure is based on a defined subjective acceptance interval around the observation data set under consideration. If the residual is greater than the rejection level introduced, the parameter realization is regarded as not being a well-suited simulator of the system, and the likelihood measure is consequently zero. If the residual is less than the rejection level, the parameter realization is accepted as a simulator of the system, and a likelihood measure is assigned. In this study a Gaussian likelihood function was used. The likelihood measure corresponds to the probability that the observation equals the simulated value—given that the residual error is Gaussian distributed, expressed by:

$$L_i = P(h_{obs,i} = h_{sim,i}) = \frac{1}{2\pi\sigma_i} e^{-RHS_i^2/2\sigma_i^2} \tag{1}$$

where L_i is the likelihood measure for the i^{th} observation, σ_i is the expected standard deviation of the groundwater head or river discharge residual, and RHS_i is the groundwater head or river discharge residual. The rejection level is set to three times the standard deviation.

The global likelihood measure

The likelihood measures, equation (1), are combined into a global likelihood measure for the simulation in question. The maximum likelihood method prescribes that the likelihood measures are multiplied:

$$L_g = \prod_{i=1}^{N} L_i = \prod_{i=1}^{N} \frac{1}{2\pi\sigma_i} e^{-RHS_i^2/2\sigma_i^2} \tag{2}$$

Here L_g is the global likelihood measure, L_i is the likelihood measure for the i^{th} observation, and N is the number of observations points.

As the number of observations increases the combined likelihood measure tends to give higher and higher weight (likelihood) to the single best simulation. As $N \rightarrow \infty$, full weight will be assigned to the single best simulation and zero weight to all other simulations.

If residuals originate from observation errors and the calibration problem is well posed, it might be reasonable to assume that the solution becomes unique as the number of observations increases.

However, the residuals derive from a number of sources; among these, errors in the conceptual model are assumed to contribute significantly.

The uncertainty arising from errors in the conceptual model does not disappear as the number of observations increases; and since the GLUE methodology is intended to represent all uncertainty in the shape of uncertainty in the parameters, the likelihood measures must be independent of, or only slightly dependent on, the number of observations.

In this study the combined likelihood measures were calculated as the geometric mean of the point likelihood measures, given by equation (3). The geometric mean ensures that all point likelihoods are greater than zero (residuals are less than the rejection level) in order to accept the simulation (L>0). The geometric mean also ensures that L is independent of the number of observations.

$$L = \sqrt[N]{\prod_{i=1}^{N} L_i} = \sqrt[N]{\prod_{i=1}^{N} \frac{1}{2\pi\sigma_i} e^{-RHS_i^2/2\sigma_{2i}^2}} \tag{3}$$

THE NUMERICAL MODEL

To solve the governing equations of groundwater, overland and river flow, a stationary, fully integrated finite difference model, based on an unstructured grid, was applied. The model was divided into five computational layers, each containing 470 elements (the horizontal discretization is illustrated in Fig. 2). The capture zone was estimated by using a particle tracking model describing advective flow (dispersion was neglected).

Particles were placed on the ground surface with a density of one per one hundred metres. The starting position of the particles that ended in the abstraction well was recorded, and the capture zone was delineated on the basis of this. All particles were transported until they reached their end positions (boundary, river or abstraction well). As indicated above, the capture zone is the surface capture zone at infinite time.

CONCEPTUAL MODELS

A synthetic set-up that contains some of the components and constraints of a real study area was constructed (Fig. 1). The study area was a 2000 m wide and 3000 m long rectangular river catchment with a 2200 m long river. The subsurface flow region consisted of an upper aquifer, an aquitard and a lower aquifer from which groundwater was abstracted. Two equally likely geological models were defined. In the first geological model (A), all three layers were extended throughout the catchment. In the second geological model (B) there was a sandy window in the aquitard within a extending over a 300 × 2000 m zone. The hydraulic conductivities in the three layers were homogeneous.

The study area was bounded by non-flow boundary conditions on the south, west and north boundaries. On the eastern boundary a constant head boundary condition was present. The net precipitation was added uniformly. Groundwater was abstracted at a constant rate of 50 mm year^{-1} (300 000 m^3 year^{-1}).

Seven head observation points were located in the lower aquifer and one river discharge observation point was located near the catchment outlet.

THE REFERENCE MODEL

For calibration purposes a reference model was constructed in order to generate the "observed" data and a reference capture zone. The geometry of this model is identical to that of the conceptual model presented in Fig 1. The second geological model (B – sandy window) was used, and the horizontal hydraulic conductivities in the upper and

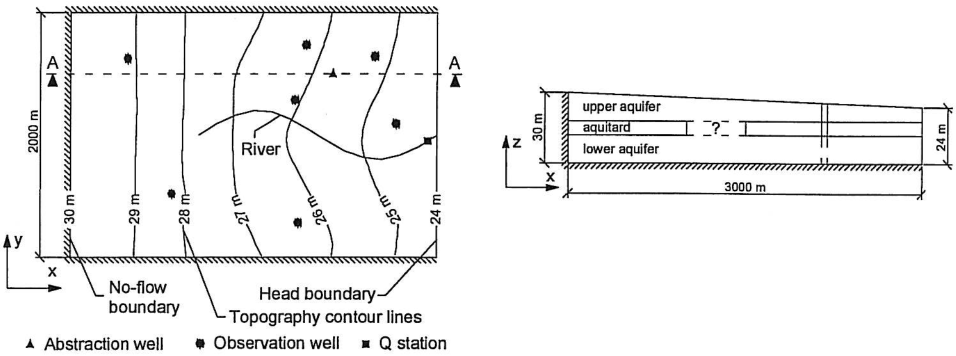

Fig. 1 Conceptual model (2000 × 3000 m).

lower aquifer and the vertical hydraulic conductivity in the aquitard were modelled as a random image within the geological layers. The purpose of modelling conductivities as random images is to introduce model errors in the conceptual description of the model area. The reference model contained geological heterogeneities that were not described in the conceptual model. This corresponds to most groundwater model applications. The random images were generated assuming lognormal conductivities with exponential decaying correlation structure.

$$\rho(h) = e^{-h/I} \tag{4}$$

where $\rho(h)$ is spatial correlation, h is the vector of distance between two points and I is integral scale.

The key parameters in the reference model are presented in Table 1. As an example the random conductivity image for the upper aquifer is illustrated in Fig. 2.

Table 1 Reference model parameters. The hydraulic conductivities are lognormal distributed, μ is mean value, σ is standard deviation and I is integral scale.

		μ	σ	I
Surface	Precipitation (mm year^{-1})	315	–	–
Upper aquifer	Horizontal conductivity (m s^{-1})	1.5×10^{-4}	7.5×10^{-5}	500
	Vertical conductivity (m s^{-1})	1.0×10^{-7}	–	–
Aquitard	Horizontal conductivity (m s^{-1})	1.0×10^{-8}	–	–
	Vertical conductivity (m s^{-1})	1.0×10^{-8}	5.0×10^{-9}	500
Lower aquifer	Horizontal conductivity (m s^{-1})	5.0×10^{-4}	2.5×10^{-4}	500
	Vertical conductivity (m s^{-1})	1.0×10^{-6}	–	–

On the basis of the reference model set-up and the numerical model described above, the reference head and river discharge data were extracted. (seven head observations in the lower aquifer and one river discharge observation).

The reference capture zone was derived from the particle flow paths presented in Fig. 3.

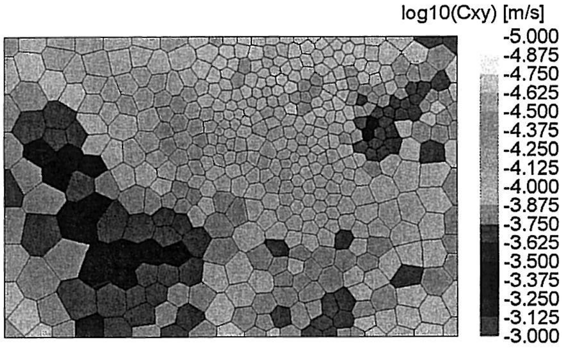

Fig. 2 Horizontal conductivity in upper aquifer (model size is 2000 × 3000 m).

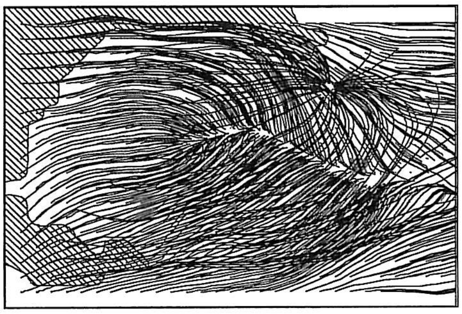

Fig. 3 The flow paths of particles and the reference capture zone (hatched) (model size is 2000 × 3000 m).

It can be seen that the river has a considerable impact on the shape and location of the capture zone. Water in the central region of the catchment drains to the river as groundwater flows in the upper aquifer, while water from the remote regions is abstracted or leaves the catchment as boundary flow. The abstracted water originates from water leached through the aquitard or the sandy window to the lower aquifer.

STOCHASTIC SIMULATION

In the conceptual model a number of key parameters are defined as being uncertain. For each of these parameters (Table 2) therefore, a likely parameter interval was constructed. The geological model was considered a discrete random variable with equal probability assigned to the two geological models. Precipitation was modelled as a uniform random variable and conductivities were modelled as $\log_{10}$ uniform random variables.

One-hundred-thousand Monte Carlo realizations of the seven random variables were generated, and for each set of parameters the flow and the particle-tracking model were executed and an upper aquifer capture zone retrieved.

Table 2 Parameter distributions used for stochastic model simulations. D, U and $L_{10}U$ denote, respectively, the deterministic, uniform and $\log_{10}$ uniform distribution.

		Distribution	Range
Geological model		U	A;B
Surface	Precipitation (mm year^{-1})	U	270 – 330
Upper aquifer	Horizontal conductivity (m s^{-1})	$L_{10}U$	$1.0 \times 10^{-5} - 5.0 \times 10^{-3}$
	Vertical conductivity (m s^{-1})	D	1.0×10^{-7}
Aquitard	Horizontal conductivity (m s^{-1})	$L_{10}U$	$5.0 \times 10^{-9} - 5.0 \times 10^{-7}$
	Vertical conductivity (m s^{-1})	$L_{10}U$	$5.0 \times 10^{-9} - 5.0 \times 10^{-7}$
Lower aquifer	Horizontal conductivity (m s^{-1})	$L_{10}U$	$1.0 \times 10^{-5} - 5.0 \times 10^{-3}$
	Vertical conductivity (m s^{-1})	$L_{10}U$	$1.0 \times 10^{-6} - 1.0 \times 10^{-4}$

RESULTS

Monte Carlo results

As a result of the Monte Carlo sampling of the parameter sets, the 100 000 capture zones obtained had, by definition, equal likelihood (weight). From a statistical analysis of the starting point of every single particle, the frequency with which the particles ended in the abstraction well could be found. The probability map in Fig. 4 was derived from an interpolation between the normalized point frequencies.

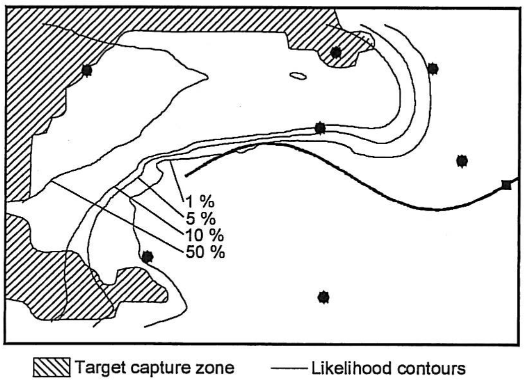

Fig. 4 Monte Carlo prediction zone. The 1% contour line encircles the area with a capture zone probability of at least 1%, etc. (model size is 2000 × 3000 m).

GLUE results

On the basis of the GLUE methodology, only the accepted simulations are considered. The likelihood measure for these simulations was calculated from equation (3). In contrast to the Monte Carlo results, where all simulations have equal likelihood (weight), the GLUE analysis results in individual likelihoods for the accepted simulations, and these likelihoods are used in the statistical analysis of the starting point of every single particle. The likelihoods are normalized so that the sum of all likelihoods is one. The point likelihoods are interpolated into a likelihood map showing the capture zone likelihood (see Fig. 6).

The likelihood measure presented in equation (1) requires an estimate of the standard deviation of the expected residuals. The expected head residuals at each head observation point were found by comparing the nodal head values from the reference model with the nodal head values from a model with uniformly distributed hydrogeological parameters within the three geological layers. The parameters were chosen so that average head residuals between the two maps were approximately equal to zero. The standard deviation of the head residuals (σ_{head}) was found to be 0.2 m. Alternatively, the standard deviation of the head residuals (σ_{head}) can be approximated from (Gelhar, 1986):

$$\sigma^2_{head} = \frac{1}{3} J^2 \sigma^2_{\ln C} I^2 \tag{5}$$

where J is the average hydrologic gradient and $\sigma_{\ln C}$ is the standard deviation of the natural logarithm of the conductivity. From equation (5) σ_{head} was estimated to be 0.18 m. The relative standard deviation on the river discharge residual (σ_{river}) was estimated to be 10%. Given these standard deviations a likelihood measure was calculated for each simulation.

The most likely simulation among those accepted was considered first. The parameter set belonging to the most likely simulation is comparable with the parameter set found from a regression analysis with the maximum likelihood objective function. The reference capture zone, the groundwater potential in the lower aquifer and the capture zone corresponding to the most likely simulation, cf. Table 3, are presented in Fig. 5. It should be noted that in this—the most likely—simulation, the predicted geological model differs from the geological model used in the reference model.

All accepted simulations were then considered. The likelihood map calculated from the 14 accepted simulations is presented in Fig. 6. The 99% prediction zone, defined as the zone with likelihood larger than 1%, covers the reference capture zone. The area of the 99% prediction zone is presented in Table 4.

Table 3 The parameter set corresponding to the most likely simulation.

		Most likely par. set	Sample range
Geological model		A	A; B
Surface	Precipitation (mm year^{-1})	309	270 – 330
Upper aquifer	Horizontal conductivity (m s^{-1})	1.88×10^{-4}	$1.0 \times 10^{-5} - 5.0 \times 10^{-3}$
	Vertical conductivity (m s^{-1})	–	1.0×10^{-1}
Aquitard	Horizontal conductivity (m s^{-1})	3.73×10^{-7}	$5.0 \times 10^{-9} - 5.0 \times 10^{-7}$
	Vertical conductivity (m s^{-1})	5.11×10^{-9}	$5.0 \times 10^{-9} - 5.0 \times 10^{-7}$
Lower aquifer	Horizontal conductivity (m s^{-1})	2.62×10^{-4}	$1.0 \times 10^{-5} - 5.0 \times 10^{-3}$
	Vertical conductivity (m s^{-1})	1.36×10^{-6}	$1.0 \times 10^{-6} - 1.0 \times 10^{-4}$

Table 4 The area of the 99% prediction zone.

Capture zone estimate	Area (m^2)	Area/Area$_{reference}$
Reference model	954 000	1.0
GLUE result	2 013 000	2.11
Monte Carlo result	3 004 000	3.15

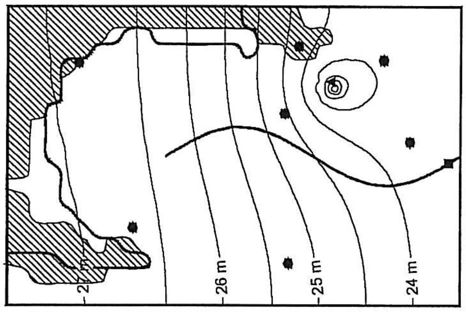

Fig. 5 Results from GLUE analysis, representing the most likely simulation (model size is 2000 × 3000 m).

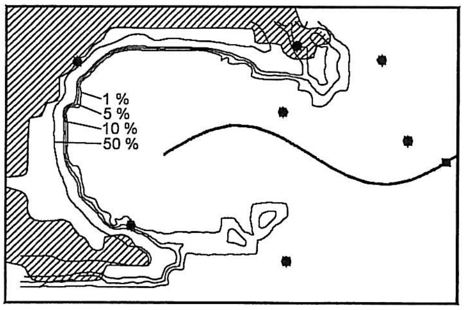

Fig. 6 GLUE prediction zone. $\sigma_{head} = 0.2$ m, $\sigma_{river} = 10\%$ (model size is 2000 × 3000 m).

From the results described above it is possible to account for model errors in the estimation of the capture zone area. Apparently a rather high prediction level has to be used to cover the reference capture zone.

In order to examine the effect of an increased degree of model error, the heterogeneity in the reference model was increased. The coefficient of variation ($V_{reference}$) used in the generation of the random conductivity images was increased from 0.5 to 1.0. The structure of the generated images was maintained so that only the amplitude of the images was changed. The standard deviation of the head residual (σ_{head}) was found to be 0.4 m and the relative standard deviation on the river discharge residual (σ_{river}) was estimated to be 20%. Figure 7 and Table 5 present the results from this case of increased heterogeneity.

Table 5 The area of the 99% prediction zone, $V_{reference} = 1.0$.

Capture zone estimate	Area (m^2)	Area/Area$_{reference}$
Reference model	954 000	1.0
GLUE result, increased heterogeneity	2 868 000	3.01
Monte Carlo result	3 004 000	3.15

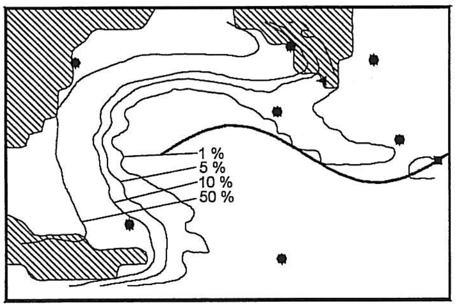

Fig. 7 GLUE prediction zone. $V_{reference}$= 1.0, σ_{head} = 0.4 m, σ_{river} = 20% (model size is 2000 × 3000 m).

It can be seen that the 99% prediction zone does not cover the reference capture zone, and the uncertainty resulting from the present degree of heterogeneity cannot apparently be accounted for.

SUMMARY AND DISCUSSION

This paper presents a method of accounting for prediction uncertainty in the estimation of capture zones within a river catchment. One of the primary objectives of the study is to evaluate the GLUE methodology for such capture zone estimations in an ill-posed model under the influence of model errors. The synthetic set-up used consists of a 6-km^2 river catchment with 3-D groundwater flow and 2-D overland flow. The groundwater zone was a three-layer system. A reference model was constructed with conductivities modelled as stochastic images, and in order to introduce model errors a conceptual model was formulated with homogeneous distributed conductivities. Two alternative conceptual geological models were presented and were estimated together with net precipitation and five hydraulic conductivities. One-hundred-thousand Monte Carlo parameter realizations were simulated and a likelihood measure calculated for each.

The single best simulation failed to predict the geological model used for the reference simulation. This reinforces the hypothesis that multiple models may be acceptable simulators of the system.

It has been shown that the reference capture zone can be predicted within the 99% prediction zone. The corresponding capture zone area is approximately twice the size of the reference capture zone.

The degree of heterogeneity was increased by raising the coefficient of variation of the conductivity by a factor of two. It was found, as expected, that this results in a decrease in predictive capability.

The study of synthetic set-ups is considered an important step towards estimating capture zones and the uncertainty linked to such estimates. It has been found very instructive to study the effect of model errors on the estimation of capture zones, especially in view of the fact that groundwater models always incorporate model errors.

Because of the large number of simulations, the method presented is computationally demanding. However, the GLUE methodology is very well suited to parallelization. The simulations presented in this paper were performed on a cluster with five 733 MHz Pentium III personal computers. The total execution time was 14 days.

The required number of simulations depends on the number of accepted simulations and hence on the acceptance level. A narrow acceptance interval will result in a smaller number of accepted simulations and the prediction may therefore be statistically uncertain. A wide acceptance interval will in general result in greater uncertainty in the prediction (since more possible solutions are accepted). There is therefore a trade-off between statistical certainty and prediction uncertainty. A small number of simulations requires wide acceptance intervals in order to produce a sufficient number of accepted simulations. A wide acceptance level will reduce the prediction capability of the model.

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