Calibration and Reliability in Groundwater Modelling: From Uncertainty to Decision Making
(Proceedings of ModelCARE'2005, The Hague, The Netherlands, June 2005). IAHS Publ. 304, 2006.

Uncertainty estimation of well catchments: combined effect of inhomogeneous transmissivity and uncertain mean recharge

FRITZ STAUFFER[1] & HARRIE-JAN HENDRICKS FRANSSEN[2]

1 *Institute of Hydromechanics and Water Resources Management, ETH -Hönggerberg, HIL G33.2, CH-8093 Zürich, Switzerland*

2 *Institute of Hydromechanics and Water Resources Management, ETH -Hönggerberg, HIL G33.3, CH-8093 Zürich, Switzerland*

stauffer@ihw.baug.ethz.ch

Abstract Steady-state catchments of pumping wells can be determined for equivalent parameters using various existing codes for groundwater modelling. The catchment boundary may be obtained by calculating the boundary path lines starting at a stagnation point in a reversed flow field. However, how uncertain is the result for heterogeneous aquifers and uncertain mean recharge? A method is proposed to estimate the uncertainty of the location of the catchment boundary in two-dimensional steady-state aquifers due to the combined effect of the uncertainty of the spatially variable unconditional transmissivity field and of the uncertain mean areal recharge rate. The former is based on the semi-analytical first-order theory, which allows estimates of the lateral second moment (variance) of the location of a moving particle. The method allows post-processing of results from groundwater modelling with respect to uncertainty estimation. In order to test the methodology it is compared with results from Monte Carlo simulations.

Keywords groundwater; protection zones; spatial variability; uncertainty estimation

INTRODUCTION

Regulations for the protection of drinking water wells require the designation of the recharge area or catchment of wells. Very often, in practice, only limited information is available for their delineation. How uncertain are well catchments resulting from deterministic groundwater modelling? Various attempts were undertaken in the past in order to answer this question using Monte Carlo type approaches, e.g. by van Leeuwen *et al.* (1998). Stauffer *et al.* (2002) formulated a first-order, unconditional semi-analytical Lagrangian method, which allows approximate evaluation of the uncertainty in the location of two-dimensional, steady-state catchments of pumping wells due to the uncertainty of the spatially variable hydraulic conductivity or transmissivity field. They applied their method successfully to a set of simple rectangular flow configurations. Stauffer (2005) reformulated the method in order to account for non-uniform recharge and non-uniform aquifer thickness in non-rectangular domains, which are often encountered in practice. This allows a post-processing of the results from standard groundwater models. Hendricks Franssen *et al.* (2002) investigated the impact of variable recharge on the characterization of well catchments using Monte Carlo type techniques. They found a much larger influence of the uncertainty in the mean recharge compared to the uncertainty due to spatial variability in recharge. In this paper we investigate an approximate approach to extend the semi-analytical Lagrangian method in order to incorporate the effect of uncertainty in mean recharge. The results for a test case are compared with those from numerical Monte Carlo simulations in order to assess the quality of the results.

IMPACT OF SPATIAL VARIABILITY IN TRANSMISSIVITY

The uncertainty in the location of the well catchment boundary is formulated along the trajectory starting at the stagnation point and proceeding upstream. The ensemble mean trajectory is determined for the flow field calculated with constant equivalent transmissivity, T_{eq}, which is approximated by the geometric mean transmissivity. Spatial variability of log-transmissivity $Y(\mathbf{x}) = \ln(T(\mathbf{x}))$ along the mean trajectory $\mathbf{s}(\mathbf{x})$ (Fig. 1) is considered by taking into account an isotropic exponential covariance function of log-transformed values with parameters describing the variance and correlation length. The lateral second moment of the particle displacements can be approximated by an integral expression (Stauffer *et al.*, 2002, 2004; Stauffer, 2005), which can be numerically evaluated. All these semi-analytical approaches make use of an empirical relationship to estimate the location uncertainty of the stagnation point. The result is an estimate of the variance of the location uncertainty $\sigma^2_{pY}(\mathbf{s}(\mathbf{x}))$ along $\mathbf{s}(\mathbf{x})$.

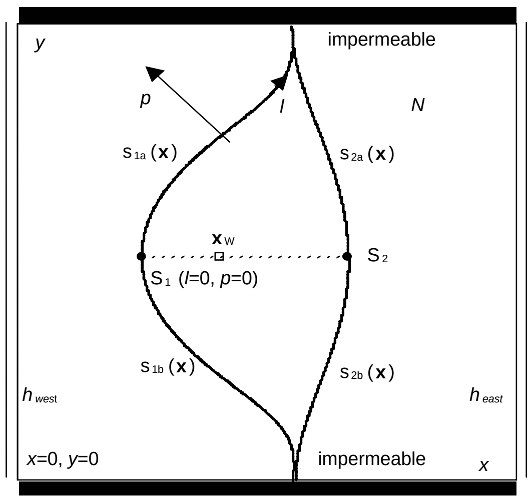

Fig. 1 Schematic catchment of a pumping well at $\mathbf{x}_w$ with constant head and impermeable boundary conditions and constant recharge rate N with solution for equivalent transmissivity; curved coordinate system p–l along catchment boundary $\mathbf{s}(\mathbf{x})$ starting at stagnation point S_1 or S_2.

IMPACT OF UNCERTAINTY IN THE MEAN RECHARGE RATE

Uncertainty due to variability in the mean recharge rate N alone can be assessed in a straightforward manner. For cases where the mean recharge rate N_{mean} can be assumed to be normally distributed, the catchment boundaries for equivalent transmissivity can be determined using standard groundwater models for the cases: (a) $N = N_{mean}$,

(b) $N_1 = N_{mean} - 2\sigma_N$ and (c) $N_2 = N_{mean} + 2\sigma_N$, where σ_N is the standard deviation of N. The symbol N_{mean} is the ensemble mean recharge rate. The trajectories $\mathbf{s}(\mathbf{x}, N)$ in case (b) and case (c) limit the 95% bandwidth of the catchment boundary due to variability in mean recharge rate N. Along the trajectory $\mathbf{s}(\mathbf{x}, N_{mean})$ the increments $p_1(\mathbf{s}(\mathbf{x}))$ and $p_2(\mathbf{s}(\mathbf{x}))$ relative to $\mathbf{s}(\mathbf{x}, N_1)$ and $\mathbf{s}(\mathbf{x}, N_2)$ can be determined.

COMBINED EFFECT

It is assumed that for a given recharge rate N the probability density function (PDF) perpendicular to the mean trajectory $\mathbf{s}(\mathbf{x}, N_{mean})$ due to variability in $Y = \ln(T)$ obeys a Gaussian distribution with mean value p' and variance σ^2_{pY} where p' is a location along the coordinate p normal to $\mathbf{s}(\mathbf{x}, N_{mean})$ with $p = 0$ on $\mathbf{s}(\mathbf{x})$ (Fig. 1). The recharge rate N itself is a Gaussian distribution with mean value N_{mean} and variance σ^2_N. It can be translated to an asymmetric PDF along p using the concept that the catchment area $A = Q/N$ can be expressed by $A = A_{mean} - B_{mean}\, p'$ with $A_{mean} = Q/N_{mean}$ assuming an unknown constant width B_{mean}. The latter can be estimated for a given location $\mathbf{s}(\mathbf{x})$ by averaging the widths B_1 and B_2 corresponding to N_1 (case b) and N_2 (case c), $B_1 = (A_1 - A_{mean})/p_1$ and $B_2 = (A_2 - A_{mean})/p_2$ using the increments $p_1(\mathbf{s}(\mathbf{x}))$ and $p_2(\mathbf{s}(\mathbf{x}))$, which are determined above. Assuming independence in the distributions $f(p)$ due to Y and N_{mean}, the combined (again asymmetric) PDF can be stated as:

$$f(p) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}\sigma_{pY}} \exp\left(-\frac{(p-p')^2}{2\sigma^2_{pY}}\right) \frac{B_{mean}}{\sqrt{\pi}\sigma_N (A_{mean} - B_{mean}\, p')^2} \exp\left(-\frac{\left(\frac{Q}{(A_{mean} - B_{mean}\, p')} - N_{mean}\right)^2}{2\sigma^2_{pY}}\right) \mathrm{d}p' \tag{1}$$

Equation (1) can be used to express the combined variance. The parameters are σ_N/N_{mean}, and p_1/p_2. The end result can be stated as follows. For the part of the perpendicular coordinate p corresponding to a recharge rate N lower than N_{mean} with $p \geq 0$ (outer part) and integration between $p' = -\propto$ and 0, the combined variance gets:

$$\sigma^2_{p,1}(\mathbf{s}(\mathbf{x})) = \sigma^2_{pY}(\mathbf{s}(\mathbf{x})) + \frac{f_1(\mathbf{s}(\mathbf{x}))\, p_1^2(\mathbf{s}(\mathbf{x}))}{4} \tag{2}$$

and for the rest of the coordinate with $p < 0$ (inner part) and integration between $p' = 0$ and $\propto$ it is:

$$\sigma^2_{p,2}(\mathbf{s}(\mathbf{x})) = \sigma^2_{pY}(\mathbf{s}(\mathbf{x})) + \frac{f_2(\mathbf{s}(\mathbf{x}))\, p_2^2(\mathbf{s}(\mathbf{x}))}{4} \tag{3}$$

The symbols f_1 and f_2 are factors, which in principle may depend on the location along the trajectory. Accordingly, separate values for the variance are estimated for each side along the mean trajectory.

MONTE CARLO SIMULATIONS

The expected location of a well catchment for inhomogeneous transmissivity and uncertain mean recharge rate is numerically analysed using a Monte Carlo based method (Gómez-Hernández & Journel, 1993). The analysis consists of the following steps:

– Multiple equally likely unconditional log-transmissivity realizations are generated.
– Multiple equally likely mean recharge rates are generated.
– The groundwater flow equation is solved for each of the generated transmissivity fields and recharge rate. In its current implementation, these equations are solved by block-centred finite differences.

For each of the realizations a particle is released at the centre of a grid cell and it is recorded whether the particle is captured by the pumping well. Averaging over the ensemble of realizations yields the probabilistic well catchment.

APPLICATION TO A TEST CASE

For comparison, the methodology was applied to a synthetic study for the catchment of a pumping well (Fig. 1). The two-dimensional rectangular domain has dimensions of 4900 × 5000 m. The northern and southern boundaries are impervious, along the western boundary a fixed head of h_{west} = 0 m is imposed, and along the eastern boundary a fixed head of h_{east} = 5 m prevails. A pumping well with pumping rate Q_w = 5000 m^3 day^{-1} is located at a distance of 1900 m from the western boundary, and 2450 m from the southern boundary. The area receives a spatially uniform recharge of N_{mean} = 1 mm day^{-1}. The variability in mean recharge rate N is σ_N/N_{mean} = 0.198. Porosity is taken as n = 0.1. Steady-state groundwater flow in a semi-confined aquifer is simulated. Geometric mean transmissivity is T_{eq} = 101 m^2 day^{-1}. The variance of $Y = \ln(T)$ is $\sigma_Y^2 = 1$ and the correlation length I_Y = 500 m. For the chosen conditions with equivalent parameters, a water divide is present along the eastern part of the area, and the well pumps water from a considerable area located west of the water divide. For the Monte Carlo simulations the domain was discretized by 50 × 50 squared grid cells of size 100 m.

The 95% uncertainty bandwidth of the catchment boundary due to spatial variability in Y only is shown in Fig. 2 for the Monte Carlo simulation and the semi-analytical approximation ($\pm 2\sigma_{pY}$). The semi-analytical approximation is not valid close to boundaries as stated in Stauffer *et al.* (2002).

The effect of uncertainty in the mean recharge rate N is depicted in Fig. 3. The 95% uncertainty bandwidth is about constant except close to boundaries. The combined effect of variability in log-transmissivity Y and in the recharge rate N is evaluated using equations (1) and (2). The factors f_1 and f_2 are found to be about 1 for the case investigated. They are determined for the stagnation point S_1 and adopted to the further locations thus making use of the observation that the ratio p_1/p_2 is about constant. This allowed simplification of the calculations. Nevertheless the approach can be easily extended in order to take into account $p_1/p_2(\mathbf{s}(\mathbf{x}))$. The uncertainty bandwidth is composed of the outer part with $p \geq 0$ and width $2\sigma_{p,1}$ and the inner part

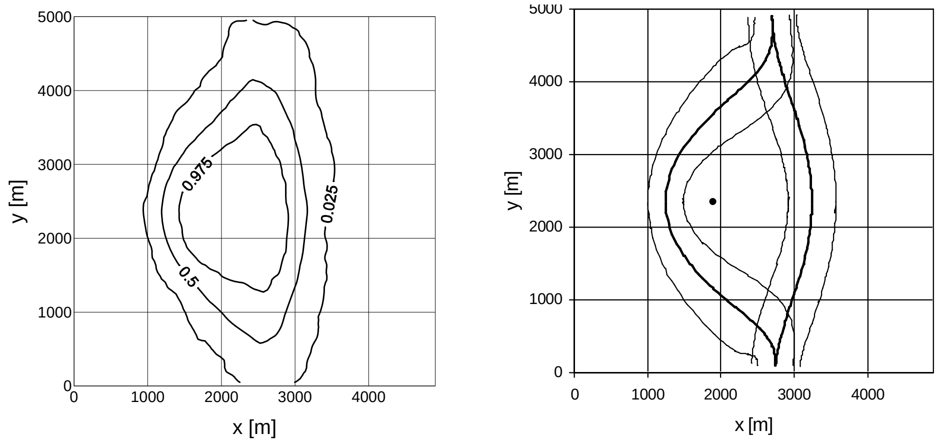

Fig. 2 Uncertainty (95%) bandwidth of the catchment boundary due to spatial variability in transmissivity only. Left: Monte Carlo simulation using 500 realizations. Right: Semi-analytical solution.

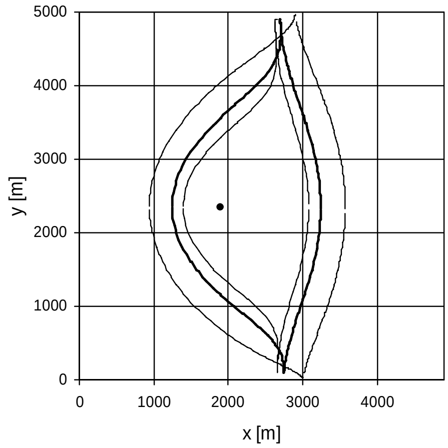

Fig. 3 Uncertainty (95%) bandwidth of the catchment boundary due to variability in mean recharge rate only with coefficient of variation of 19.8%. Semi-analytical solution.

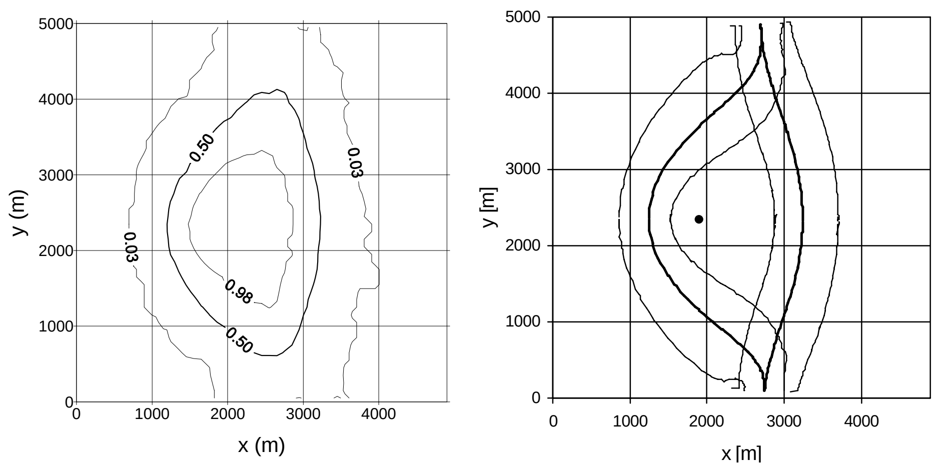

Fig. 4 Uncertainty (95%) bandwidth of the catchment boundary due to combined effects of spatial variability in transmissivity and variability in mean recharge with coefficient of variation of 19.8%. Left: Monte Carlo simulation using 100 realizations. Right: Semi-analytical combined solution.

with $p < 0$ and width $2\sigma_{p,2}$. The result of the simulation is shown in Fig. 4. Again, the solution is not valid close to boundaries.

DISCUSSION AND CONCLUSIONS

An approximate method is proposed to estimate the uncertainty of the location of the catchment boundary of a pumping well in a two-dimensional steady-state aquifer due to the combined effect of the uncertainty of the spatially variable unconditional log-transmissivity field $Y(\mathbf{x})$ and of the uncertain mean areal recharge rate $N(N_{mean}, \sigma^2_N)$. The former is based on the semi-analytical first-order theory, which allows estimates of the lateral second moment (variance) of the location of a moving particle along the mean trajectory $\mathbf{s}(\mathbf{x})$. The concept consists of the assumption that the combined effect can be evaluated in the normal direction p to the mean trajectory $\mathbf{s}(\mathbf{x}, N_{mean})$. The effect of variability in the mean recharge rate N for equivalent transmissivity can be assessed by simple groundwater modelling. Since the two contributions are assumed to be independent, the probability density function of the combined effect can be stated. This leads to a simple evaluation of the combined variance of the location uncertainty along the catchment boundary. As can be seen from the test case the result of the proposed method is in fair correspondence to the result of numerical Monte Carlo simulations except close to boundaries. The main attraction of the proposed method is the much smaller computational demand compared with numerical Monte Carlo techniques. Similar concepts can in principle be formulated for further cases like the impact of the location uncertainty of a boundary segment of the flow domain (characterized by a variance), again in combination with spatial variability in $Y(\mathbf{x})$.

Acknowledgements This study was performed within the European Research Project "Stochastic Analysis of Well Head Protection and Risk Assessment" (W-SAHaRA). The project was supported by the Swiss Federal Office for Education and Science (BBT), project 99.0543.

REFERENCES

Gómez-Hernández, J. J. & Journel, A. G. (1993) Joint sequential simulation of multi-Gaussian fields. In: *Geostatistics Troia'92*, vol. 1 (ed. by A. Soares), 85–94. Kluwer Academic Publishers, Dordrecht, The Netherlands.

Hendricks Franssen, H.-J., Stauffer, F. & Kinzelbach, W. (2002) Impact of spatio-temporally variable recharge on the characterization of well capture zones. In: *Calibration and Reliability in Groundwater Modelling: A Few Steps Closer to Reality* (edited by K. Kovar & Z. Hrkal) (Proc. ModelCARE'2002, Prague, Czech Republic), 470–477. IAHS Publ. 277. IAHS Press, Wallingford, UK.

Stauffer, F., Attinger, S., Zimmermann, S. & Kinzelbach, W. (2002) Uncertainty estimation of well catchments in heterogeneous aquifers. *Water Resour. Res.* **38**, doi:10.1029/2001WR000819.

Stauffer, F., Hendricks Franssen, H.-J. & Kinzelbach, W. (2004) Semi-analytical uncertainty estimation of well catchments: conditioning by head and transmissivity data. *Water Resour. Res.* **40**, doi: 10.1029/2004WR003320.

Stauffer, F. (2005) Uncertainty estimation of pathlines in ground water models. *Ground Water* **43**(6), 843–849, doi:10.1111/j.1745-6584.2005.00054.x.

van Leeuwen, M., te Stroet, C. B. M., Butler, A. P. & Tompkins, J. A. (1998) Stochastic determination of well capture zones. *Water Resour. Res.* **34**(9), 2215–2223.