Delineation of source protection zones using statistical methods — Source link

Fritz Stauffer, Alberto Guadagnini, Adrian P. Butler, Harrie-Jan Hendricks Franssen ...+4 more authors

Institutions: ETH Zurich, Polytechnic University of Milan, Imperial College London, Delft University of Technology

Published on: 01 Apr 2005 - Water Resources Management (Kluwer Academic Publishers)

Topics: Aquifer and Groundwater recharge

Delineation of Source Protection Zones Using Statistical Methods

Author(s):
Stauffer, Fritz; Guadagnini, Alberto; Butler, Adrian; Hendricks Franssen, Harrie-Jan; Van De Wiel, Neeltje; Bakr, Mahmoud; Riva, Monica; Guadagnini, Laura

Publication date:
2005-04

Permanent link:
https://doi.org/10.3929/ethz-b-000032663

Originally published in:
Water Resources Management 19(2), https://doi.org/10.1007/s11269-005-3182-7

Water Resources Management (2005) 19: 163–185
DOI: 10.1007/s11269-005-3182-7

Delineation of Source Protection Zones Using Statistical Methods

FRITZ STAUFFER[1,*], ALBERTO GUADAGNINI[2], ADRIAN BUTLER[3], HARRIE-JAN HENDRICKS FRANSSEN[1], NEELTJE VAN DE WIEL[4], MAHMOUD BAKR[3], MONICA RIVA[2] and LAURA GUADAGNINI[2]
[1]*Federal Institute of Technology (ETH), Zurich, Switzerland;* [2]*Politecnico di Milano, D.I.I.A.R., Milan, Italy;* [3]*Imperial College of Science, Technology and Medicine, London, U.K.;* [4]*Delft University of Technology, The Netherlands*
(**author for correspondence, e-mail: stauffer@ihw.baug.ethz.ch; Fax: +41 44 6331061*)

(Received: 16 March 2004; in final form: 2 July 2004)

Abstract. Source protection zones are increasingly important for securing the long-term viability of drinking water derived from groundwater resources. These may be either time-related capture zones or catchments related to the activity of a pumping well or spring. The establishment of such zones is an indispensable measure for the proper assessment of groundwater resource vulnerability and reduction of risk, which may be induced by human activities. The delineation of these protection zones is usually performed with the aid of models, which are in turn based on site-specific information of the aquifer's geometry, hydraulic parameters and boundary conditions. Owing to the imperfect knowledge of such information, predicting the location of these zones is inherently uncertain. It is possible to quantify this uncertainty in a statistical manner through the development of probability maps, which shows the probability that a particular surface location belongs to the aquifer's capture zone (or catchment area). This publication aims at the investigation of the requirements for the establishment of probabilistic source protection zones, the practical use of stochastic methods in their delineation, and the use of data-assimilation for uncertainty reduction. It also provides a methodology for the implementation of these methods by modelling practitioners.

Key words: groundwater, modelling, protection zones, statistical methods, stochastic methods, uncertainty estimation

1. Introduction

Owing to the technical, legal, social and financial difficulties, which can arise from restoring contaminated groundwater, it is obvious that the timely protection of aquifers is preferable. Regulations for the protection of drinking water wells usually require the delineation of areas that define a prescribed minimum groundwater residence time and the entire catchment area of the well. On the one hand there are existing or planned activities, which represent hazards or risks for a particular groundwater resource, and on the other hand, the aquifers exhibit a certain degree of vulnerability to a wide range of chemical and biological pollutants. Basic elements for the protection of groundwater from the point of view of water quality are:

- *Well/spring capture zone (time-related)*: Normally it is required that the residence time of any groundwater or pollutant should exceed a prescribed value (e.g., 50 days according to the regulations on water resources protection of Germany and many other countries, 10 days in the Swiss regulation). The idea behind this regulation is that pathogenic microbes are generally eliminated within this time span, and that in the case of hazards there would be enough time for interventions (abstraction of polluted water, establishment of hydraulic barriers) or other remediation measures.
- *Well/spring recharge area*: Any groundwater within this zone, and therefore any pollutant, would eventually reach the well, provided the flow field within this zone is at steady state. Regulations for the protection of water resources require the designation of recharge areas of pumping wells, which are endangered by pollution. An example is the delineation of the recharge area required by the Swiss regulation on the protection of water resources. The recharge area is related to the well/spring catchment or wellhead protection zone. Springs are normally treated in a similar way as wells.

Necessary measures and restrictions with respect to land use and restrictions of human activities within established protection zones are defined by the regulations. The protection of aquifers should be accompanied by a monitoring of the piezometric head and of the groundwater quality by an appropriate network of observation wells and periodical sampling. To assess the yield and potential capacity of groundwater resources, and to calculate the extent of the capture zones and contaminant travel times, the flow and transport characteristics of the aquifer are needed. This also includes an assessment of the temporal development (seasonal development, long-term development) of the groundwater flow. The work presented in this paper contains conclusions from the project W-SAHaRA "Stochastic Analysis of Well Head Protection and Risk Assessment" (funded by the European Commission during the period 2000–2003). Such conclusions concern a comparative analysis of the stochastically based methodologies, which can be used in the delineation of protection zones in unconsolidated aquifers. Moreover, they concern the formulation of requirements for the establishment of probabilistic groundwater protection zones, the practical use of stochastic methods in delineating protection zones, and the data-assimilation process in the stochastic analysis of protection zones.

2. General Procedure for the Delineation of Protection Zones

The following types of groundwater protection zones are considered here: the time-related capture zone of a well, and the recharge area of a well. Well capture zones for a prescribed groundwater residence time can be determined by evaluating the corresponding isochrones, which are the contour lines of equal groundwater residence time. These isochrones can be calculated analytically for a system of wells in a uniform base flow (e.g., Bear and Jacobs, 1965). They can also be computed numerically for arbitrarily shaped flow fields (Kinzelbach *et al.*, 1992), for example, by back-tracking a fluid particle starting at the well until the prescribed residence time is reached. Well catchments can be determined numerically by back tracking a fluid particle starting near the stagnation point of the well. In both cases the detailed velocity field is required, assuming that advection is the dominant process. For the evaluation of the velocity field the following parameters and conditions are generally required:

1. The flow geometry: This information is obtained from hydrogeological investigations. The prevailing flow field can often be approximated by a horizontal two-dimensional (2D) flow and transport model. Moreover, compared to three-dimensional (3D) flow the formulation and numerical implementation of 2D models is usually much simpler than in the 3D case. Nevertheless, it should be kept in mind that 3D effects may be important in practice. For instance, the evaluation of a 3D capture zone or catchment, at least in the vicinity of the well, is (in principle) required when dealing with partially penetrating or partially screened pumping wells.
2. The pumping rate of the well: The given or planned schedule of the pump should be taken into account.
3. The groundwater recharge rate: The rate is estimated on the basis of hydrological considerations.
4. The infiltration rate from rivers and creeks: The rate can be estimated on the basis of hydrological considerations, or by calibration of a flow model using nearby head and/or concentration data.
5. The levels of the bottom and of the top of the aquifer formation: This information is generally obtained from borehole and/or geophysical investigations.
6. The piezometric head of the aquifer: This information is generally obtained from boreholes and/or geophysical investigations.
7. The location of the boundary of the flow domain to be investigated: This information is obtained from a regional hydrogeological and hydrological investigation. The boundaries are often chosen in such a manner that a feasible formulation of the boundary conditions (fixed head or streamline) can be obtained.
8. The boundary conditions: This information consists of the heads at the boundary (or portions of it) or of the water flux through the boundary (or portions of it). This information can be obtained from hydrological and hydrogeological investigations.
9. The hydraulic conductivity (or transmissivity) of the aquifer: This information can be obtained from pumping test evaluation or other procedures.
10. The porosity of the aquifer: This information is relevant for proper isochrones prediction and can be deduced, for instance, from tracer tests.

3. Impact of Parameter Uncertainty

Relatively small capture zones can usually be determined in a reasonable manner using the above stated principles. However, problems arise for larger capture zones or recharge areas due to the impact of parameter uncertainty. Evers and Lerner (1998) asked the question "How uncertain is our estimate of a wellhead protection zone?" Therefore, the above list of parameters and conditions should be discussed in a qualitative manner with respect to the associated parameter uncertainty:

1. The extent of the flow domain is subject to uncertainty, mainly due to the extrapolation and interpolation of data.
2. The pumping rate of the well is probably the less uncertain of all information. Often, long-term averaged pumping rates can be used. However, the pumping schedule can affect the capturing mechanism by the well by the time-dependent velocity field.
3. The groundwater recharge rate can, in general, only be indirectly determined. It depends on the rainfall rate, on the evaporation and transpiration rate, and on the subsequent flow processes in the unsaturated zone. Overall, the recharge rate is time dependent and more or less spatially variable. Often these effects can hardly be assessed precisely. Even the temporally and spatially averaged recharge rate may show considerable uncertainty.
4. The infiltration rate from rivers, creeks, and lakes is difficult to assess since it cannot be measured directly, in general. It depends on the local infiltration conditions, which can be affected by clogging. The rate is in general time dependent and spatially variable.
5. The level of the bottom and the top of the aquifer are usually based on local borehole information and can be obtained by interpolation. Consequently, some uncertainty remains. The situation may be improved by a combination of geophysical techniques.
6. The piezometric head of the aquifer is based on local borehole measurements and represents valuable data used for a calibration of the flow model. The piezometric head essentially dominates the flow directions. Consequently, transient effects in the head field can be of utmost importance. It is usually vertically averaged information while in some cases can be known at different intervals along a vertical.
7. The location of the boundary of the aquifer is based on a regional hydrogeological and hydrological assessment and is always subject to uncertainty.
8. Fixed head boundary conditions are subject to uncertainty caused by data interpretation and interpolation. The transient behaviour of these conditions can hardly be assessed in detail. Flux boundary conditions are also difficult to estimate. They can often be determined in a satisfactory manner with the help of flow models, provided that reliable data of hydraulic conductivity and piezometric head are available. Nevertheless, some uncertainty inevitably remains. The averaged value and the transient behaviour of both types of boundary conditions can be important for the flow field, and, therefore, for the location of the capture zone or catchment.

9. Hydraulic conductivity always shows a more or less pronounced spatial variability due to the heterogeneous nature of aquifers. Therefore, a thorough investigation of the field scale hydraulic conductivity is advisable. The local values can never be known in detail everywhere. Spatial variability can considerably affect the uncertainty of the location of the capture zone or catchment. In addition, the scale at which the measurements have been taken has to be carefully considered in the evaluation of the measurement.
10. Aquifer kinematic porosity directly affects the flow velocity and therefore the residence times, which subsequently determines the location of the capture zone. Moreover, a spatial variability of field scale and local porosity may also exist in unconsolidated aquifers. However, the effect of a spatial variability can be smaller than that of the hydraulic conductivity.

Many of the above listed items concern local information, which is typically measured in boreholes. Therefore, the quality of the overall information in a particular flow domain very much depends on the spatial and/or temporal density of the available data. However, due to economic and logistic reasons, the information is often sparse. The location of data points is normally restricted to particular regions within the aquifer. Similarly, the temporal frequency of measurements is often limited. Moreover, experimental data are sometimes corrupted by measurement and interpretive errors. Overall, the combined effects of the uncertainty of all parameters and conditions can considerably affect the precision of the calculated capture zone or catchment. For small areas a more simplified and intuitive assessment of the uncertainty is often possible, which can be taken into account in the delineation of the protection zone. However, for larger areas the uncertainty can be quite large. Depending on the economical and ecological importance of the protection zone, the implications of the degree of uncertainty associated with its predicted location can be prohibitive. Therefore, methods are needed to quantify the uncertainty and provide guidance in the acquisition of site data to reduce it. In general, uncertainty can be reduced by increasing investigations (borehole investigations, parameter estimation, etc.). However, since resources are limited the task should consist of a methodological approach, which is pragmatic in the sense that it optimises efficiency. Consequently, there is a need for knowledge and tools, which enable a conceptual and quantitative assessment of the impact of parameter uncertainty on the location of existing or planned protection zones.

The consequence of the uncertainty of the essential parameters, which determine capture zones or catchments of a pumping well, is that the location of these zones cannot be determined with certainty. Therefore, the location of the protection zones can only be defined in a statistical manner. Consequently, the best we can do is to offer a probability map, rendering the probability with which a particular location belongs to the capture zone or catchment. Such concepts can be fed directly into a risk-assessment of a particular groundwater resource.

4. Importance of Data in the Analysis of Well Protection Zones

The uncertainty about the location and the extent of protection zones can generally be reduced by an increase of direct measurements (for example, by increasing the amount of hydrogeological data, such as hydraulic conductivity, or direct measurements of state variables, such as piezometric head). Furthermore, geological data from field investigations (such as borehole descriptions, cone penetration tests, etc.) can, in principle, also be used to constrain predictions, resulting in a global reduction of uncertainty in the delineation of protection zones. The most important hydrogeological data are listed in Section 2. These data may be used:

- To establish deterministic flow and transport models of the aquifer. Here, we use the wording "deterministic" in order to identify a model, which does not provide, by its nature, a quantification of uncertainty associated to predictions other than by means of a traditional sensitivity analysis. Deterministic models, based on calibrated averaged parameters (using the concept of equivalent parameters for different aquifer zones), are often obtained using various manual or automated optimisation procedures.
- To deterministically delineate protection zones of pumping wells for various conditions (boundary conditions, pumping rates, recharge conditions, etc.), using the calibrated flow and transport models. However, a considerable uncertainty may remain; the latter cannot be quantified, by definition, via the use of a deterministic model.
- To evaluate the statistical and stochastic parameters characterising spatial variability.
- To establish a stochastic model (Section 5) based on the deterministic (i.e., certain, or known with rather reasonable certainty) and stochastic parameters, forcing terms and boundary conditions.

5. Modelling Spatial Variability and Uncertainty of Variables

The uncertainty of the parameters may be on the one hand due to measurement errors inherent in a specific evaluation method, and on the other hand due to the more or less strong spatial variability of many parameters, like hydraulic conductivity $K(\mathbf{x})$, which can never be known in detail everywhere. A viable way out of the dilemma may be, for example, to cast the problem in a probabilistic framework and considering the aquifer as one of many stochastic realisations. Stochastic variables such as hydraulic conductivity do not behave like a white noise but show a distinct spatial correlation structure with the correlation between two values, depending on their distance. This correlation structure can be described by, e.g., a two-point (auto-) covariance function. A further important feature is the probability density function of the parameter under consideration.

A common approach in the practical application of prediction models is to formulate equivalent parameters, thus replacing the real heterogeneous system by a homogeneous equivalent model (e.g., Renard and de Marsily, 1997). Therefore, one task consists of finding adequate equivalent parameters, such as equivalent hydraulic conductivity, as a function of quantities investigated.

The investigation of the impact of spatial variability of flow parameters concerns the evaluation of the expected (mean) location (first statistical moment) of the capture zone or catchment and its associated variance (second statistical moment). Such moments can be theoretically based on the ensemble of all equally possible heterogeneous realisations of the considered aquifer, honouring some sets of measured data. The formulation of second moments is referred below by the use of moment equations (Section 7). Widespread numerical procedures to the solution of this problem are, for example, Monte Carlo-based techniques (Section 6), in which space-dependent or also time-dependent parameter values of numerical models are generated in a statistical manner, followed by a subsequent (numerical) solution and analysis of each of the corresponding deterministic systems. Usually, the following statistical or geostatistical parameters are required for a stochastic method:

- The stochastic variable(s), e.g., the hydraulic conductivity $K(\mathbf{x})$, or its natural log-transformed counterpart, $Y(\mathbf{x}) = \ln(K(\mathbf{x}))$.
- The probability density function, *pdf*, of the stochastic variable: This is often approximated by a normal or a log-normal probability distribution. For log-normally distributed variables, a log-transform of the variable is applied.
- The ensemble mean value of the stochastic variable, e.g., $\langle Y(\mathbf{x})\rangle$, or the geometric mean value, K_g.
- The variance of the stochastic variable, e.g., σ_Y^2; and the related standard deviation.
- The two-point covariance function $C_Y(\mathbf{x}_1, \mathbf{x}_2)$. Often, a particular and convenient invariant covariance model is selected to express the spatial correlation, e.g., the exponential covariance model $C_Y(\mathbf{x}_1, \mathbf{x}_2) = \sigma_Y^2 \exp(-|\mathbf{x}_1 - \mathbf{x}_2|/s_Y)$, where the correlation length, I_Y, has to be evaluated on the basis of available data.

When considering randomness in more than one parameter, cross-correlations or cross-covariance amongst different parameters might be needed. The parameters have to be evaluated *a priori*, based on measurements or on experience. For spatially distributed variables, like hydraulic conductivity, a variogram analysis (de Marsily, 1986) may be used.

6. Use of Monte Carlo Techniques

Monte Carlo (MC) techniques are general and versatile tools that allow one or several parameters of a model to be uncertain. The idea is to generate many realisations of synthetic aquifer flow (and eventually transport) models in such a manner that they reflect the observed (experimental) parameter uncertainty. The results are subsequently analysed in a statistical manner to quantify the uncertainty inherent in the expected result. However, MC techniques are often very time consuming and it is not always clear what number of realisations is necessary for the convergence of the method (e.g., Ballio and Guadagnini, 2004). Nevertheless, they represent rather general and versatile tools for the investigation of ranges of spatially variable parameters in the context of both linear and non-linear problems.

Consider a randomly heterogeneous flow domain, where, for simplicity, we assume the hydraulic conductivity, $K(\mathbf{x})$, to be the only source of uncertainty, and the objective is to condition prediction and associated uncertainty to both hydraulic conductivity and head measurements. For this domain a log-transformed hydraulic conductivity field $Y(\mathbf{x}) = \ln(K(\mathbf{x}))$ is generated (realisation i), conditional to hydraulic conductivity measurements in boreholes. Statistics of Y to be employed as input to the generation process are usually derived from the available data set and are a critical aspect of the entire procedure. The corresponding flow field is then calculated using a forward numerical model and the computed hydraulic heads are compared with available measured hydraulic head values. The misfit between the model predictions and the measurements can be used to obtain a better estimate of the hydraulic conductivity field using a numerical inverse modelling technique, thus effectively conditioning the i-th realisation of the MC process on the available hydraulic head data. The ensemble of the results of all realisations ($i = 1, \ldots, N_{\mathrm{MC}}$) is then statistically analysed in order to obtain predictions and quantify the uncertainty of the expected results. Solving the inverse groundwater flow and/or transport model for each realisation is many times more intensive in computing time than solving the forward flow and/or transport model and the computational time increases with the number of conditioning data. A possible procedure for applying conditional MC techniques to delineate well protection zones (or catchments) under steady state-flow conditions can be summarised as follows:

1. Generation of N_{MC} realisations (e.g., $N_{\mathrm{MC}} = 500$) of a random log-transformed hydraulic conductivity field $Y_i(\mathbf{x}) = \ln(K_i(\mathbf{x}))(i = 1, \ldots, N_{\mathrm{MC}})$, conditional to available $K_j(\mathbf{x}_j)$ data at locations $\mathbf{x}_j$, where $j = 1, \ldots, N_K$ (see below), N_K being the number of conditioning K measurements.
2. Solution of the groundwater flow problem for each of the realisations $K_i(\mathbf{x})$ using a numerical inverse modelling technique, conditional to head data $h_k(\mathbf{x}_k)$, with $k = 1, \ldots, N_h$ or other type of data (see below). This results in updated realizations $K_i(\mathbf{x})$. Alternatively, conditioning on $h_k(\mathbf{x}_k)$ data can also be performed simultaneously with $K_j(\mathbf{x}_j)$ data.
3. For each flow field $h_i(\mathbf{x})$ one or several idealised tracer particle are released at each grid cell of a regular grid. Numerical particle tracking is performed to calculate the well capture zone (for the given residence time) or the well catchment for each realisation using an advective transport model. The end points of all particles are recorded.
4. The statistical analysis of the ensemble of particle trajectories over all N_{MC} realisations provides the probability distribution $P(\mathbf{x})$ of the capture zone or the

catchment. In other words, one obtains a map showing the spatial distribution of the probability P that a fluid particle (or idealised tracer particle) released at a particular location $\mathbf{x}$ is captured by the well within the requested residence time, or the probability P that a particular location $\mathbf{x}$ belongs to the catchment.

Codes to generate random hydraulic conductivity fields $Y(\mathbf{x}) = \ln(K(\mathbf{x}))$ investigated by the authors during this work, were SGSIM (Deutsch and Journel, 1998) FGEN (Robin *et al.*, 1993), GSTAT (Pebesma, 1999), or GCOSIM3D (Gómez-Hernández and Journel, 1993). GCOSIM3D is a follow-up version of SGSIM. It enables a better reproduction of the covariance function $C_Y(\mathbf{x}_1, \mathbf{x}_2)$, especially in case of long correlation lengths I_Y.

The groundwater flow equation can be solved, for instance, with the finite difference code MODFLOW (McDonald and Harbaugh, 1988) and forward particle tracking can be performed using the computer code MODPATH (Pollock, 1994), whereby at least one particle is released at each grid cell.

One of the stochastic inverse modelling techniques investigated in this work is the Sequential Self-Calibrated Method (Gómez-Hernández *et al.*, 1997; Hendricks Franssen, 2001) for the inverse modelling of groundwater flow and mass transport, conditioned to hydraulic conductivity and head data. The method can also handle (in principle) transient head data with the joint estimation of spatially variable hydraulic conductivity and storativity fields and is formulated in three dimensions. The method has been extended to estimate jointly hydraulic conductivities and recharge (Hendricks Franssen *et al.*, 2004a).

Another investigated inverse modelling technique is the Method of Representers (Valstar, 2001). This inverse algorithm considers spatially variable parameters explicitly. It can use both hydraulic head and concentration data to reduce the uncertainty of model parameters for three-dimensional, quasi-steady flow regimes. For conditioning on head measurements the Method of Representers has been implemented into MODFLOW (Van de Wiel *et al.*, 2002, 2004) and in a modified version of the finite element code S-InvMan (Bakr, 2000). It has also been used to examine the worth of head and concentration data on groundwater remediation using the pump-and-treat method (Bakr *et al.*, 2003).

The accuracy of the numerical estimate of the probability $P(\mathbf{x})$ that a location $\mathbf{x}$ belongs to a capture zone or catchment strongly depends on the number of Monte Carlo runs, N_{MC}, and therefore on the convergence of the method. A minimum number N_{MC} for which the estimated value of $P(\mathbf{x})$ is practically independent of N_{MC} has to be identified. Van Leeuwen (2000) suggests that, at least in two dimensions, approximately $N_{\text{MC}} = 500$ realisations normally result in an acceptable convergence, and that the convergence after about 1000 realisations hardly improves.

For illustration, the results of an unconditional Monte Carlo analysis aimed at the evaluation of the catchment of a well is shown in Figure 1. At the western boundary a constant head boundary condition was applied. The remaining boundaries

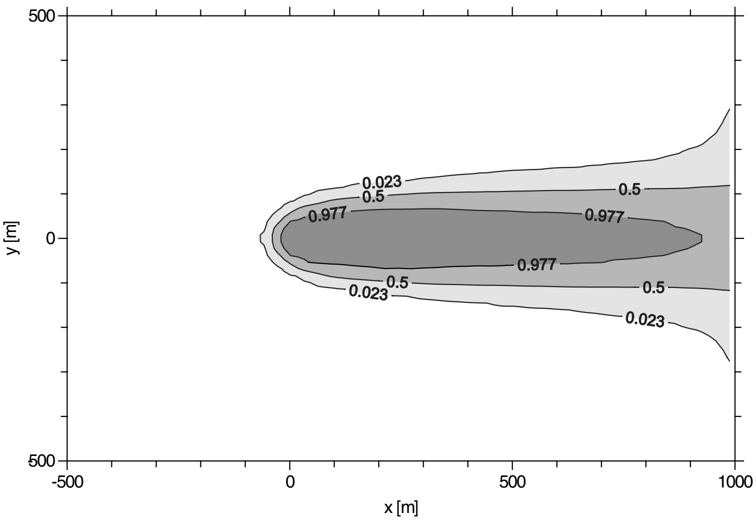

Figure 1. Probability map of a well catchment; Monte Carlo results. The well is located at $x = 0$, $y = 0$.

were chosen as impermeable. The geometric mean hydraulic conductivity K_g was 10 m/day, the variance σ_Y^2 was 0.1, the correlation length $I_Y = 50$ m, adopting an exponential covariance function for Y. The pumping rate was 200 m^3/day and the recharge rate 1 mm/day. The number of Monte Carlo runs was $N_{\mathrm{MC}} = 1000$. The map shows the probability $P(\mathbf{x})$ that a fluid particle at a given location $\mathbf{x}$ reaches the well.

Further numerical or analytical Monte Carlo techniques to deduce capture zones or catchments in a statistical manner were suggested, e.g., by Kunstmann and Kinzelbach (2000), Franzetti and Guadagnini (1996), Guadagnini and Franzetti (1999), Van Leeuwen *et al.* (1999), Wheater *et al.* (2000), Hunt *et al.* (2001), Feyen *et al.* (2001), Jacobson *et al.* (2002), or Feyen *et al.* (2003a). In addition, Van Leeuwen *et al.* (1999) have used Monte Carlo analysis to evaluate the impact of uncertainty in the location of drift overlying a production aquifer on well capture zones at Wierden, The Netherlands.

7. Use of Moment Equations

A major conceptual disadvantage of Monte Carlo approaches is that they do not provide a theoretical insight into the nature of the solution. Therefore, there is a need for alternative approaches. One method is based on the use of moment equations.

A complete first-order (in the variance of Y) stochastic mathematical formalism that allows to obtain an estimate of the travel time and the trajectory (rendered by the first moments) together with the associated prediction errors (rendered by their second moments) for idealised tracer particles advected in a randomly heterogeneous aquifer has been derived (Guadagnini *et al.*, 2003; Riva *et al.*, 2004) and compared against numerical Monte Carlo simulations the formalism, solute particles are injected at a single point and travel along a (random) trajectory towards a given discharge point or line. Travel time mean and variance are functions of first and second moments and cross-moments of trajectory and velocity components. Trajectory mean and variance are functions of the statistical moments of the components of the velocity field. The equations were developed from a consistent first-order expansion in σ_Y^2. As such, they are nominally limited to mildly non-uniform fields, with $\sigma_Y^2 < 0.5$, or more heterogeneous fields, in the presence of conditioning. The work has been developed in two dimensions and the extension to a more general three-dimensional scenario is straightforward. Furthermore, procedures were developed, which allow conditioning of the statistical moments of the flow field and, therefore, of travel time moments, on hydraulic heads measurements and/or aquifer architecture (e.g., Hernandez *et al.*, 2003; Winter *et al.*, 2003).

Stauffer *et al.* (2002) investigated the uncertainty in the location of two-dimensional, steady state catchments of pumping wells due to the uncertainty of the spatially variable hydraulic conductivity field by a semi-analytical Lagrangian technique. For the analysis it is assumed that the aquifer can be modelled as a steady-state horizontal, confined or unconfined system. The well discharge rate and the recharge rate are constant. The uncertainty bandwidth of the catchment boundary is approximated at first order (in the variance of Y) by formulating the transversal second moment of the tracer particle displacements along the expected mean boundary of the catchment, starting at the stagnation point in a reversed velocity field. A special approach is suggested for the estimation and conditioning of uncertainty in the location of the stagnation points. For illustration, the results for the estimated catchment boundary of a well together with its uncertainty bandwidth is shown in Figure 2. The conditions were the same as in Figure 1. A similar Langrangian approach for time-related capture zones in heterogeneous aquifers without recharge was presented by Lu and Zhang (2003).

Bakr and Butler (2004b) have used an alternative numerical approach, in which the original partial differential equation of flow and advective transport, is first discretised on a specified grid using finite elements, and then the resulting equation, the so-called space–time equation, is used to derive the statistical moments of the flow and mass transport quantities. The approach is based on a Taylor's series approximation of the discrete system of equations and is often termed the vector space-state/adjoint state approach.

8. Impact of Recharge Uncertainty

The spatial variability of hydraulic conductivity is usually believed to be the main contributor to the uncertainty in the estimation of a well catchment and, therefore, its effects have been intensively studied (see, e.g., references cited above). The impact of the spatially variable recharge on the estimation of a well catchment is

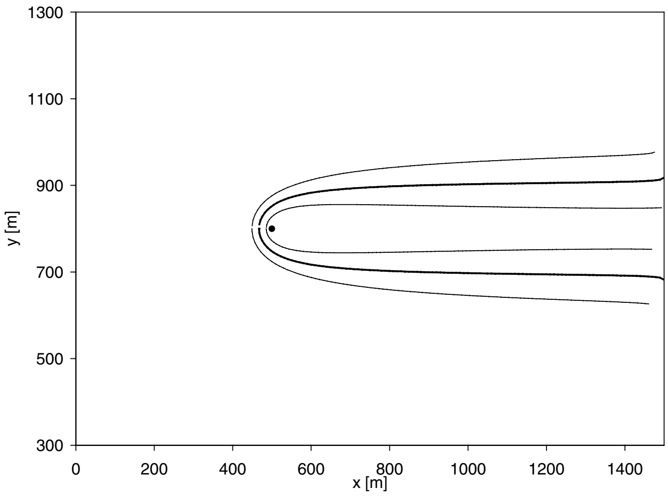

Figure 2. Uncertainty bandwidth (mean and 95% probability) of the location of a well catchment boundary estimated by the Lagrangian semi-analytical method (Stauffer *et al.*, 2002)

known to a lesser extent. In this case, the relevant question to be answered relates to whether recharge uncertainty does contribute significantly to the well catchment uncertainty in case there is at the same time a considerable spatial variability of hydraulic conductivity. In addition, another source of uncertainty may be the temporal variability of recharge.

The recharge uncertainty has been subjected to a synthetic study (Hendricks Franssen *et al.*, 2002). The study focused on a flow regime that is typical for a humid, temperate climate. The average yearly recharge is chosen as 360 mm and the seasonal variations in precipitation are not very strong. Furthermore, the aquifer materials have a relatively high permeability. The main practical conclusions from the Monte Carlo type study were:

- The spatial variability of recharge has only a limited impact on the uncertainty of the well catchment. The impact is larger in case of a larger recharge correlation length. However, even in case of large recharge correlation length and unrealistically large spatial recharge variability, its influence on the well catchment is very limited for moderately heterogeneous hydraulic conductivity fields ($\sigma_Y^2 \approx 1$). It is expected that for a moderately or strongly heterogeneous hydraulic conductivity field, the spatial variability of recharge is overruled by the spatial variability of hydraulic conductivity.
- Nevertheless, the uncertainty in the mean recharge has an important impact on the well catchment uncertainty, also in case of a moderately or even strongly heterogeneous hydraulic conductivity field. For recharge it is therefore important to estimate the uncertain mean, while the detailed estimation of the spatially variable patterns of recharge is normally not needed. It may be necessary to

estimate the mean areal recharge for multiple zones in case there is evidence of varying means between different areas (as is the case for differences in land use).

- The temporal recharge variability can be important to consider in some specific situations. In case the groundwater residence time in the catchment is not clearly longer as compared to the time scale on which the recharge fluctuates, it may be necessary to investigate time series of recharge. In humid, temperate climate zones the variations between years are normally limited. However, the recharge varies significantly over a year. Normally a recharge minimum in summer and early autumn and a recharge maximum in winter and early spring is reached. In case the expected groundwater residence time in the catchment is not clearly larger than one year, effects of temporal recharge variability may be expected.

9. Impact of Uncertainty in Geostatistical Parameters, Average Hydraulic Conductivity, and Boundary Conditions

In most of the studies in stochastic subsurface hydrogeology the covariance function $C_Y(\mathbf{x}_1, \mathbf{x}_2)$ and the geometric mean hydraulic conductivity K_g are assumed to be known exactly. In practice, they are estimated from a limited number of hydraulic conductivity data. As a consequence, these estimates are associated with a considerable uncertainty. A further important source of uncertainty, which normally is not addressed in hydrogeological studies, is related to the boundary conditions. The location of the boundaries and the prescribed flux or prescribed head values on the boundaries are normally assumed known.

The impact of the mentioned sources of uncertainty was tested in a synthetic study (Hendricks Franssen *et al.*, 2004b). The studied two-dimensional domain had extensions of 5×5 km. The northern and southern boundaries were impervious and along the western and eastern boundaries fixed heads of respectively 0 and 5 m were imposed. A pumping well was located 500 m west of the domain centre. The area received a spatially uniform recharge of 363 mm/year. Steady-state groundwater flow in an aquifer with constant thickness was simulated. A hydraulic conductivity field was generated with a mean value of 102 m/day and an exponential covariance function C_Y with a variance of $\sigma_Y^2 = 1$, and a correlation length of $I_Y = 500$ m (1/10 of the domain). This reference field was considered as unknown reality of the study. As a consequence, a water divide along the eastern part of the area was present and the well pumps water from a considerable area located west of the water divide. Figure 3 shows the corresponding reference well catchment. The reference hydraulic conductivity field was sampled 100 times by selecting 10 measurements each. From the selected 100 random data sets 100 different mean hydraulic conductivity values and 100 different covariance functions of $Y = \ln(K)$ were estimated. The impact of these uncertainties on the estimation and estimated variance of the hydraulic conductivity field, the hydraulic head field and the catchment zone were quantified. The following practical conclusions could be drawn from this study:

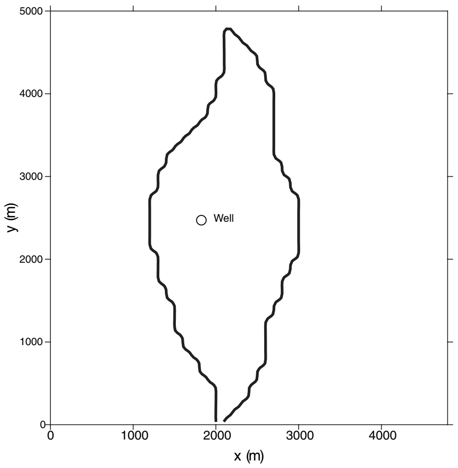

Figure 3. Reference well catchment of the synthetic study for the investigation of the impact of uncertainty in covariance function C_Y, the geometric mean hydraulic conductivity K_g, and the boundary conditions (Hendricks Franssen *et al.*, 2004).

1. The uncertainty in the mean hydraulic conductivity, e.g., K_g, had a very limited influence on the characterisation of the hydraulic conductivity field, the hydraulic head field and the catchment zone.
2. The uncertainty in the hydraulic conductivity covariance function $C_Y(\mathbf{x}_1, \mathbf{x}_2)$ had a slightly larger impact on the characterisation of the hydraulic head field, the hydraulic conductivity field and the catchment zone than the uncertainty in the mean hydraulic conductivity, but was nevertheless quite small. However, this conclusion is valid only for the ensemble mean over all 100 samples of measurements. For the case that just one set of measurements is taken, as is of course the case in practical situations, the impact of the uncertainty of the covariance function can be much more pronounced.
3. The uncertainty with respect to piezometric head values on prescribed head boundaries had a large effect on the characterisation of the hydraulic head field, the hydraulic conductivity field and the catchment zone.
4. Inverse modelling (conditioning to error-free piezometric head data) was able to reduce the impact of the above mentioned three sources of uncertainty.

Note that the conclusions from the synthetic study cannot necessarily be generalised to any other case.

10. Sampling Design and Monitoring Strategies

Incorporation of measurement data through conditioning is a requirement for reducing uncertainty in the location of the well capture zone or catchment. However, the success of this conditioning depends on the type of measurement, the amount and spatial pattern of the measurements and the measurement error (Bakr and Butler, 2003; Hendricks Franssen and Stauffer, 2004; Van de Wiel *et al.*, 2004). Furthermore, the conditioning performance seems to be dependent on the type of aquifer (confined or unconfined), the correlation length I_Y and variance σ_Y^2 and the well pumping rate (Van Leeuwen *et al.*, 2000; Bakr and Butler, 2003; Van de Van de Wiel *et al.*, 2002).

Extensive Monte Carlo-based analyses on the effect of hydraulic conductivity (or transmissivity) data and piezometric head observations (both separately and combined) in reducing capture zone uncertainty enabled to provide a set of basic rules about location and type of data and for the development of optimal measurement strategies for uncertainty reduction. The effect of conditioning is primarily measured in terms of the reduction in the width of the capture zone's probability distribution.

In general, uncertainty related to well capture zones or catchments decreases with increasing incorporation of hydraulic conductivity and hydraulic head data (conditioning density). However, the conditioning effect for different sampling schemes with similar amounts of measurement data can be quite different. What is the relative worth of different types of measurements? Synthetic case studies indicate the greater importance of hydraulic conductivity measurements over head data in reproducing the reference well capture zone (Bakr and Butler, 2004a; Feyen *et al.*, 2003a). It appears that it is not possible to get satisfactory results using head measurements alone, especially in highly heterogeneous aquifers (for $\sigma_Y^2 > 1$). Although head measurements are capable of estimating hydraulic gradient quite accurately, they do not contain sufficient information on the variation of hydraulic conductivity which, in turn, leads to high variability in pore water velocity and hence the well capture zone location. Furthermore, results show that a combination of both head and hydraulic conductivity data can reduce the width of the capture zone distribution more significantly than either type of data alone (Bakr and Butler, 2004a). Feyen *et al.* (2003a) concluded that head observations are more effective in reducing the width of the capture zone distribution, whereas hydraulic conductivity measurements are more valuable in predicting the actual location of the unknown capture zone. Feyen *et al.* (2003b) also incorporated tracer arrival times, hydraulic conductivity measurements and hydraulic head observations in the stochastic capture zone delineation. Their evaluation indicates that travel time data seem to be effective in reducing the overall uncertainty and to some extent in revealing large irregularities in the shape of the capture zone. In general, the incorporation of tracer and solute concentration enhances the aquifer characterisation and the accuracy of flow and transport predictions, since such data are complementary to head and conductivity measurements (Medina and Carrera, 1996; Valstar, 2001; Hendricks Franssen *et al.*, 2003).

Observation network of head and/or hydraulic conductivity measurements can be optimised in a systematic manner. Such methodologies can also provide a way to minimise the number of sampling locations, required to reduce capture zone uncertainty to an acceptable level. Van de Wiel *et al.* (2004) investigated several strategies for selecting the optimal additional location for a piezometric head observation in a synthetic confined aquifer with a single pumping well. The strategies are: (a) selecting the location, where the head variance is highest; or (b) selecting the location where the sum of covariances between head at that location and at the other potential measurement locations is largest; or (c) selecting the location that minimises the head variances summed over the model domain; or (d) selecting the location where the reduction in capture zone uncertainty is highest. The last strategy clearly showed the best results in reducing the capture zone uncertainty. However, it is also the most time intensive, whereas the three other criteria do not require Monte Carlo simulations. Among these three design strategies, the strategy that minimised the summed head variance performed poorly in terms of minimisation of capture zone uncertainty in case of a relatively small number of selected head measurements.

Hendricks Franssen and Stauffer (2004) proposed optimisation procedures for selecting new locations for both head and hydraulic conductivity data in a synthetic confined aquifer with spatially uniform recharge and a single pumping well. The algorithm enables to place additional measurement locations nearly optimally. The true optimum can hardly be found since only a limited number of possible combinations of new measurement locations can be analysed realistically, since computation of all possible combinations, even for a few additional measurements, is extremely time consuming. Two selection criteria were implemented: (a) the minimisation of the expected average log-transformed hydraulic conductivity variance, and (b) the minimisation of the average hydraulic head variance. It was found that both strategies were successful. However, the differences between the optimal strategies and heuristic criteria, where the sampling points are distributed evenly over the whole aquifer, were small. This indicates that covering the domain of interest regularly with a measurement network is a close to optimal strategy in characterising the general flow field. However, selecting measurement locations in zones with a capture probability of about $0.05 < P(\mathbf{x}) < 0.95$ seems to be a better option for characterising a well catchment. Nevertheless, there is a trade-off between continuing adding measurement points in these zones and placing additional locations in the areas around the uncertain zones.

11. Application to a Field Case

Many of the methodologies developed for the stochastic characterisation of well capture zones and catchments have been intensively tested in several synthetic numerical simulations. The next logical step was to apply these methodologies in a real world case study. For this purpose the Lauswiesen test site in the Neckar valley near the city of Tuebingen in southwest Germany was selected. This site has been intensively studied before and during the W-SAHaRA project (Sack-Kühner, 1996; Martac *et al.*, 2003a, 2003b) including stochastic inverse modelling. For the

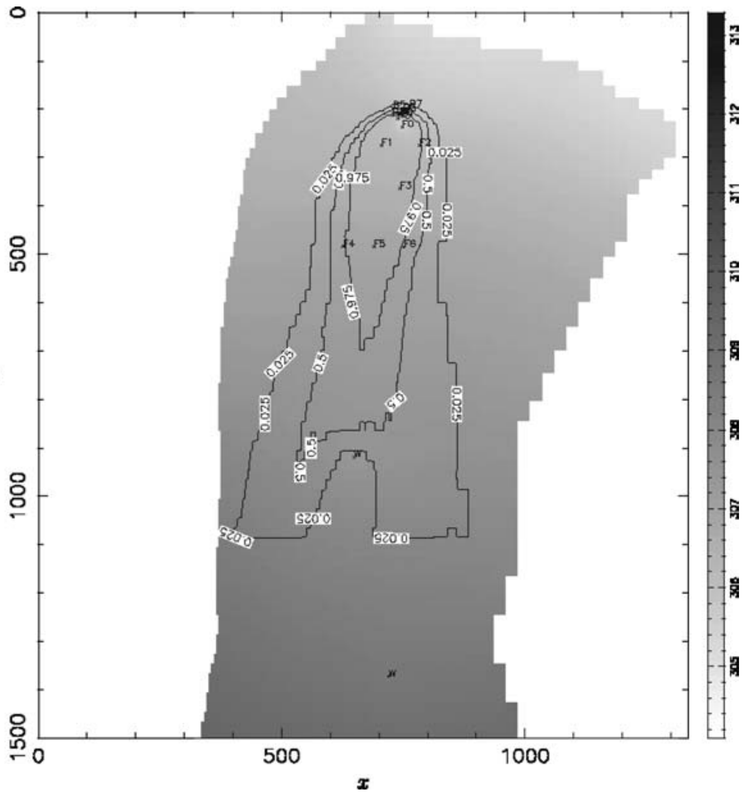

Figure 4. Lauswiesen field case: Map of ensemble averaged hydraulic head (m) and the probabilistic 50 days well capture zone of abstraction well F0 calibrated for the pumping stage. Locations of head measurements (H) and injection wells (F1–F6) are marked. Dark grey represents a high value for hydraulic head.

sake of illustration, Figure 4 shows the estimated 50 days well capture zone for the Lauswiesen site during the tested pumping conditions, using a Monte Carlo approach based on the Representer Method. The main conclusion from this field case is that the stochastic methodologies are indeed capable of yielding reasonable stochastic estimates of the well capture zone or catchment. However, as compared with a synthetic case there exist several implications that point to the need for further research and development. In a synthetic test case the performance of an algorithm can be easily evaluated in a systematic manner. In practice one would like to use all available information, but then no data are available anymore to test how well the model predictions performed. Although detailed verification is in general not possible in practice, it is desirable to exclude some data and/or tests from the conditioning procedures and to use them for comparison with the model predictions. In the present test case we found that the model predictions do not deviate too much from the experimental results. The peak arrival time for three tracers was quite well predicted. It can be stated that the results are generally compatible with the tracer tests. The most important conclusions were:

- We found that the role of the river, and its interaction with the aquifer was crucial. Measured time series of groundwater and Neckar river levels indicate that the river level has a major impact on the hydraulic head distribution in the aquifer. Errors in modelling this boundary condition prohibit a more reliable characterisation of the aquifer hydraulic conductivity and of the capture zone. In order to directly handle the inverse stochastic modelling of river–aquifer interactions in an adequate and concise manner, further research is needed. In addition, in order to enable a successful inverse stochastic simulation of the river–aquifer flow conditions more measurement locations along the river are needed.
- The estimation of the hydraulic conductivity covariance function had to be based on sparse data only. This was a further main source of uncertainty.
- It was shown that inverse modelling is to a certain degree able to correct the estimation error.
- Data from sieve analysis (soft information) allowed a more realistic reconstruction of the spatial distribution of aquifer hydraulic properties (Martac *et al.*, 2003).

The practical case of the Lauswiesen field site shows that there is a need for inverse modelling procedures that can handle three-dimensional aquifers with a large number of grid cells and transient flow conditions. In this sense, parallelisation of Monte-Carlo type models can lead to an improvement in their performance. Ye *et al.* (2004) recently presented a comparative analysis, in terms of runtimes, of the computational efficiencies of parallel algorithms used in the context of recursive Moment Equation and Monte Carlo methods. In addition, the models should be able to condition to tracer test information on a routinely basis in order to further improve the predictions.

12. Conclusions

A result of incomplete knowledge of the essential parameters that determine well capture zones or catchment areas is that the location of these zones/areas cannot be determined with certainty, since the amount of available data is always limited. In particular, the location of data points is often restricted to specific regions within the aquifer (due to economic and logistic reasons). Furthermore, experimental data are always corrupted to some degree by measurement and interpretive errors. Consequently, the location of the protection zones can only be defined in statistical manner and should therefore, be represented using a probabilistic catchment/capture zone map (as illustrated in Figures 1, 2 or 4). This provides us the probability $P(\mathbf{x})$, with which a particular location $\mathbf{x}$ belongs to the capture zone or well catchment (Section 3). This requires a stochastic analysis for well capture zone and catchment. The general procedure is depicted in Figure 5. The probabilistic capture zone or

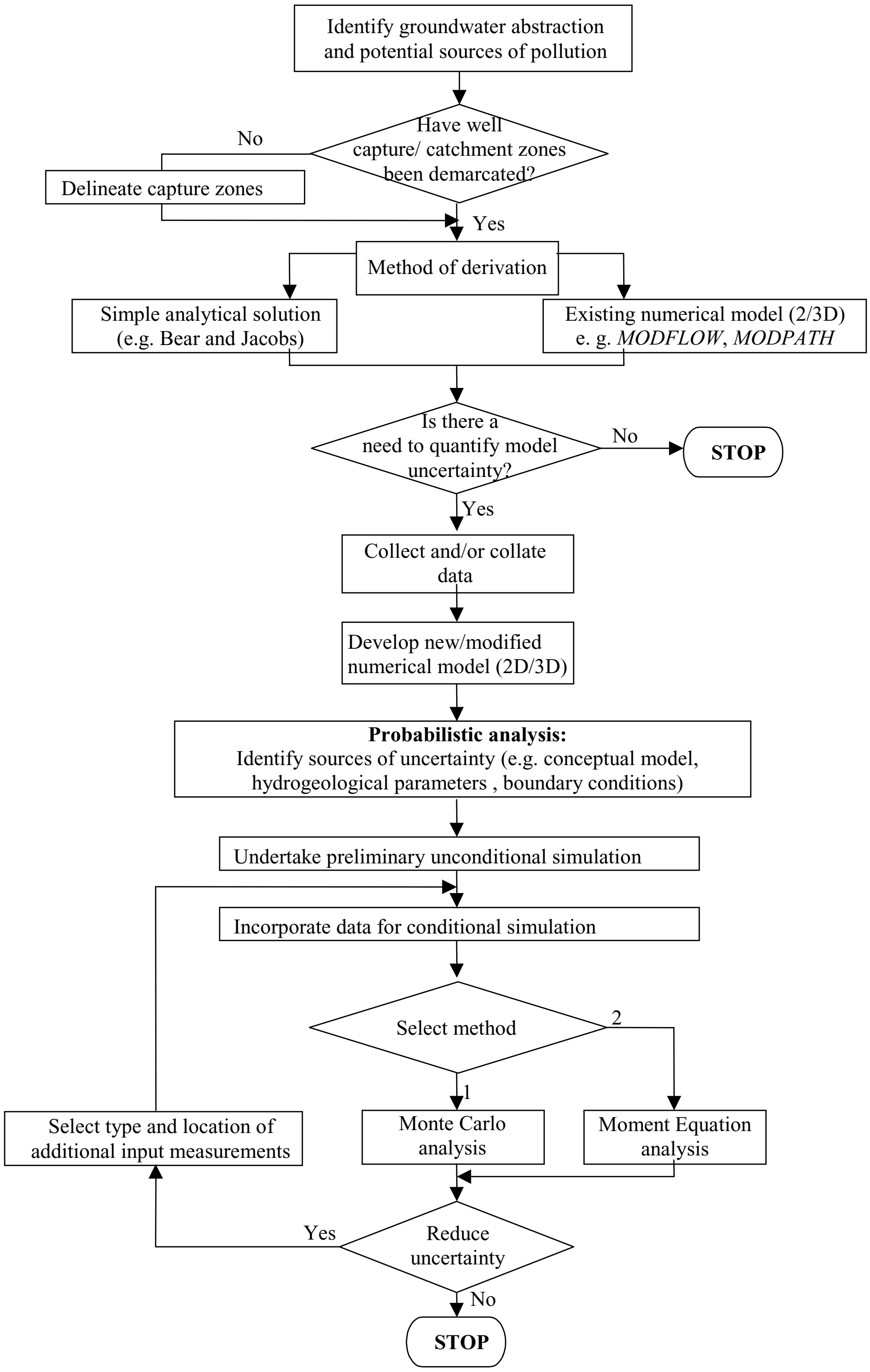

Figure 5. Stochastic analysis of well capture zones or catchments.

catchment map of a pumping well can then directly be used by the decision maker for the delineation of the protection zone, based on specific political, ecological, and/or economical reasons. Moreover, such a probabilistic representation naturally fits with the requirements for a risk-based assessment that are frequently required in groundwater management decisions.

The development and evaluation of methods and tools to produce stochastic capture zone/catchment maps of pumping wells was the main task of the work undertaken by the authors within the EC-funded project W-SAHaRA. The selection of a specific method for a stochastic analysis of protection zones of pumping wells depends on specific conditions, as the dimension of the flow problem, the flow geometry, the aquifer type (confined, unconfined, multi-aquifer system), the recharge conditions, the number of wells, the spatial variability of hydraulic conductivity, and the type, number and location of conditioning data.

The methodologies that characterise capture zones and catchments stochastically have reached the stage that they can be applied in practice, but further development is needed so that they can be applied more routinely. Semi-analytical Lagrangian methods without conditioning on measured data (Stauffer *et al.*, 2002) are in many practical studies an option to get a quick "idea" of the uncertainty of a well catchment. They have the advantage that they need relatively little computing time. One of the few special requirements would be the estimation of a reliable hydraulic conductivity covariance function. Expert knowledge is needed to estimate such a covariance function. In case of only few measurements, multiple calculations with different covariance functions are possible, and not very time consuming. More general, methods based on moment equations, conditional to measurements, have shown their potential for interesting future applications. Numerical Monte Carlo type methods are already well developed for flow problems. They tend to be more flexible and can for example handle cases with a large log-transformed hydraulic conductivity variance and may also handle strongly non-linear systems. In addition, in case of inverse modelling they can also treat systems with various sources of uncertainty jointly, like hydraulic conductivities, spatial and temporal recharge and various boundary conditions.

The focus of this work has been primarily targeted at unconsolidated porous media. Although fractured rock systems have not been specifically considered, the techniques developed here may also be applied where such systems are treated as equivalent porous media.

Acknowledgements

The study was performed within the European research project "Stochastic Analysis of Well Head Protection and Risk Assessment" (W-SAHaRA), Contract No. EVK1-CT-1999-00041. The project has been supported by the Swiss Federal Office for Education and Science (BBT), project 99.0543.

References

Bakr, M. I., 2000, 'A Stochastic Inverse-Management Approach to Groundwater Quality Problems', *Ph.D. thesis*, Delft University of Technology, Delft, The Netherlands.

Bakr, M. I. and Butler, A. P., 2004a, 'Worth of head data in well capture zone design, deterministic and stochastic analysis', *J. Hydrol.* **290**(3–4), 202–216.

Bakr, M. I. and Butler, A., 2004b, 'Nonstationary stochastic analysis in well capture zone design using first-order Taylor's series approximation', *Water Resour. Res.* (submitted).

Bakr, M. I., te Stroet, C., and Meijerink, A., 2003, 'Stochastic groundwater quality management; role of spatial variability and conditioning', *Water Resour. Res.* **39**, 2078, doi: 10.1029/2002WR001745.

Ballio, F., and Guadagnini, A., 2004, 'Convergence assessment of numerical Monte Carlo simulations in groundwater hydrology', *Water Resour. Res.* **40**, W04603, doi:10.1029/2003WR002876.

Bear, J. and Jacobs, M., 1965, 'On the movement of water bodies injected into aquifers', *J. Hydrol.* **3**, 37–57.

Deutsch, C. V. and Journel, A. G., 1998, *GSLIB: Geostatistical Software Library and User's Guide*, 2nd ed., Oxford University Press, New York.

Evers, S. and Lerner, D. N., 1998, 'How uncertain is our estimate of a wellhead protection zone?', *Ground Water* **36**, 49–57.

Feyen, L., Beven, K. J., De Smedt, F., and Freer, J., 2001, 'Stochastic capture zone delineation within the generalized likelihood uncertainty estimation methodology: Conditioning on head observations', *Water Resour. Res.* **37**, 625–638.

Feyen, L., Ribeiro, P. J. Jr., Gómez-Hernández, J. J., Beven K. J., and De Smedt, F., 2003a, 'Bayesian methodology for stochastic capture zone delineation incorporating transmissivity measurements and hydraulic head observations', *J. Hydrol.* **271**, 156–170.

Feyen, L., Gómez-Hernández, J. J., Ribeiro Jr., P. J., Beven, K. J., and De Smedt, F., 2003b, 'A Bayesian approach to stochastic capture zone delineation incorporating tracer arrival times, conductivity measurements and hydraulic head observations', *Water Resour. Res.* **39**, 1126, doi: 10.1029/2002WR001544.

Franzetti, S. and Guadagnini, A., 1996, 'Probabilistic estimation of well catchments in heterogeneous aquifers', *J. Hydrol.* **174**, 149–171.

Gómez-Hernández, J. J. and Journel A. G., 1993, 'Joint simulation of MultiGaussian random variables', in A. Soares (ed.), *Geostatistics Tróia 92*, vol. 1, Kluwer Academic Publishers, pp. 85–94.

Gómez-Hernández, J. J., Sahuquillo, A., and Capilla, J. E., 1997, 'Stochastic simulation of transmissivity fields conditional to both transmissivity and piezometric data. 1. Theory', *J. Hydrol.* **203**, 162–174.

Guadagnini, A. and Franzetti, S., 1999, 'Time-related capture zones for contaminants in randomly heterogeneous formations', *Ground Water* **37**, 253–260.

Guadagnini, A. Sànchez-Vila, X., Riva, M., and De Simoni, M., 2003, 'Mean travel time of conservative solutes in randomly heterogeneous unbounded domains under mean uniform flow', *Water Resour. Res.* **39**, 1050, doi: 10.1029/2002WR001811.

Hendricks Franssen, H. J. W. M., 2001, 'Inverse Stochastic Modelling of Groundwater Flow and Mass Transport', *Ph. D. thesis*, Technical University of Valencia.

Hendricks Franssen, H. J. W. M., Stauffer F., and Kinzelbach, W., 2002, 'Impact of spatio-temporally variable recharge on the characterisation of well capture zones', in K. Kovar and Z. Hrkal (eds.) *ModelCARE 2002—Calibration and reliability in Groundwater Modelling: A Few Steps Closer to Reality*, IAHS Publication, 227, pp. 470–477.

Hendricks Franssen, H. J. W. M., Gómez-Hernández, J.J. and Sahuquillo, A., 2003, 'Coupled inverse modelling of groundwater flow and mass transport and the worth of concentration data', *J. Hydrol.* **281**, 281–295.

Hendricks Franssen, H. J. W. M. and Stauffer, F., 2004, 'Optimal design of measurement networks for groundwater flow predictions', *Adcances in Water Resour.* (submitted).

Hendricks Franssen, H. J. W. M., Stauffer, F., and Kinzelbach, W., 2004a, 'Joint estimation of transmissivities and recharges—Application: Stochastic characterization of well capture zones', *J. Hydrol.* **294**, 87–102.

Hendricks Franssen, H. J. W. M., Stauffer F., and Kinzelbach, W., 2004b, 'Influence of uncertainty of mean transmissivity, transmissivity variogram and boundary conditions on estimation of well capture zones', in Sanchez-Villa, X., Carrera, J., and Gómez-Hernández, J. J. (eds.), *GeoEnv IV-Geostatistics for Environmental Applications*, Kluwer Acad. Publ., pp. 223–234.

Hernandez, A. F., Neuman, S. P., Guadagnini, A., and Carrera, J., 2003, 'Conditioning mean steady state flow on hydraulic head and conductivity through geostatistical inversion', *Stoch. Environ. Res. Risk Assessm.* **17**, 329–338.

Hunt, R. J., Steuer, J. J., Mansor, M. T. C., and Bullen, T. D., 2001, 'Delineating a recharge area for a spring using numerical modeling, Monte Carlo techniques, and geochemical Investigation', *Ground Water* **39**, 702–712.

Jacobson, E., Andricevic, R., and Morrice, J., 2002, 'Probabilistic capture zone delineation based on an analytic solution', *Ground Water* **40**, 85–95.

Kinzelbach, W., Marburger, M. and Chiang, W.-H., 1992, 'Determination of groundwater catchment areas in two and three spatial dimensions', *J. Hydrol.* **134**, 221–246.

Kunstmann, H. and Kinzelbach, W., 2000, 'Computation of stochastic wellhead protection zones by combining the first-order second-moment method and Kolmogorov backward equation analysis', *J. Hydrol.* 237, 127–146.

Lu, Z. and Zhang, D., 2003, 'On stochastic study of well capture zones in bounded, randomly heterogeneous medi', *Water Resour. Res.* **39**, 1100, doi10.1029/2002WR001633.

Marsily de, G., 1986, *Quantitative Hydrogeology*, Academic Press, Orlando, FL.

Martac, E., Sack-Kühner, B. and Ptak, T., 2003a, 'Multilevel—Multitracer Tests in Heterogeneous Porous Aquifers: A Method for Subsurface Investigation and Testing of Stochastic Models for the Delineation of Wellhead Protection Zones', *Proceedings of 8th International FZK/TNO Conference on Contaminated Soil*, Gent, Belgium.

Martac, E., Guadagnini, L., Riva, M. and Ptak,T., 2003b, 'Multivariate Geostatistical Parameterization Approach for 3D Transient Stochastic Modeling of Wellhead Protection Zones in a Highly Heterogeneous Aquifer', *Proceeding of MODFLOW and MORE 2003 Understanding Through Modelling*, Poeter *et al.*, International Ground Water Modeling Center (IGWMC), Colorado School of Mines, pp. 686–690.

McDonald, M. G. and Harbaugh, A. W., 1988, 'A Modular Three-Dimensional Finite-Difference Groundwater Flow Model', *Manual 83–875*, U.S. Geological Survey.

Medina, A. and Carrera, J., 1996, 'Coupled estimation of flow and solute transport parameters', *Water Resour. Res.* **32**, 3063–3076.

Pebesma, E., 1999, 'GSTAT User's manual', Technical Report, Department of Physical Geography, Utrecht University, Utrecht, The Netherlands.

Pollock, D. W., 1994, 'User's guide for MODPATH/MODPATH-PLOT, Version 3: A Particle Tracking Post-Processing Package for MODFLOW, the U.S. Geological Survey Finite-Difference Ground-Water Flow Model', *Open-File Report*, U.S. Geological Survey, pp. 94–464.

Renard, P. and de Marsily, G., 1997, 'Calculating equivalent permeability: A review', *Adv. Water Resour.* **20**, 253–278.

Riva, M., Sanchez-Vila, X., De Simoni, M., Guadagnini, A., and Willmann, M., 2004, 'Effect of heterogeneity on aquifer reclamation time', in Sanchez-Villa, X., Carrera, J., and Gómez-Hernández, J. J. (eds.), *GeoEnv IV-Geostatistics for Environmental Applications*, Kluwer Acad. Publ., pp. 259–270.

Robin, M. J., Gutjahr, A. L., Sudicky, E. A., and Wilson, J. L., 1993, 'Cross-correlated random field generation with the direct Fourier transform method', *Water Resour. Res.* **26**, 2385–2397.

Sack-Kühner, B. T., 1996 'Einrichtung des Naturmessfeldes "Lauswiesen Tuebingen", Erkundung der hydraulischen Eigenschaften, Charakterisierung der Untergrundheterogenitaet und Vergleich der Ergebnisse unterschiedlicher Erkundungsverfahren', *Diploma Thesis*, Fachbereich Geowissenschaften, Eberhard-Karls-University Tuebingen, Germany.

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

Valstar, J. R., 2001, 'Inverse Modeling of Groundwater Flow and Transport', *Ph.D. Thesis*, Delft University of Technology, The Netherlands.

Van de Wiel, N. P. A. J., Gehrels, J. C., te Stroet, C. B. M. and Valstar, J. R., 2002, 'Optimally Reducing Uncertainty in Well Capture Ones using Hydraulic Head Data', in K. Kovar, Z. Hrkal (eds.), *ModelCARE 2002—Calibration and Reliability in Groundwater Modelling: A Few Steps Closer to Reality*, IAHS Publication, 277, pp. 498–507.

Van de Wiel, N. P. A. J., Gehrels, J. C., te Stroet, C. B. M., and Valstar, J. R., 2004, 'Conditioning stochastic well capture zones on optimised grids of head measurements', *J. Hydrol.* (Submitted).

Van Leeuwen, M., 2000, 'Stochastic determination of Well Capture Zones Conditioned on Transmissivity Data', *Ph.D. thesis*, Imperial College of Science, Technology and Medicine, London.

Van Leeuwen, M., Butler, A. P., te Stroet, C. B. M., and Tompkins, J. A., 1999, 'Stochastic Determination of the Wierden (Netherlands) Capture Zones', *Ground Water* **37**, 8–17.

Van Leeuwen, M., Butler, A. P., te Stroet, C. B. M., and Tompkins, J. A., 2000, 'Stochastic determination of well capture zones conditioned on regular grids of transmissivity measurements', *Water Resour. Res.* **36**, 949–957.

Wheater, H. S., Tompkins, J. A., van Leeuwen, M., and Butler A. P., 2000, 'Uncertainty in groundwater flow and transport modelling — a stochastic analysis of well protection zones', *Hydrol. Processes* **14**, 2019–2029.

Winter, C. L., Tartakovsky, D. M., and Guadagnini, A., 2003, 'Moment differential equations for flow in highly heterogeneous porous media', *Surveys in Geophysics* **24**, 81–106.

Ye, M., Neuman, S. P., Guadagnini, A., and Tartakovsky, D. M., 2004, 'Nonlocal and localized analyses of conditional mean transient flow in bounded, randomly heterogeneous porous media', *Water Resour. Res.* **40**, W05104, doi: 10.1029/2003, WR002099.