An integrated approach for addressing uncertainty in the delineation of groundwater management areas

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ABSTRACT

Uncertainty is a pervasive but often poorly understood factor in the delineation of wellhead protection areas (WHPAs), which can discourage water managers and practitioners from relying on model results. To make uncertainty more understandable and thereby remove a barrier to the acceptance of models in the WHPA context, we present a simple approach for dealing with uncertainty. The approach considers two spatial scales for representing uncertainty: local and global. At the local scale, uncertainties are assumed to be due to heterogeneities, and a capture zone is expressed in terms of a capture probability plume. At the global scale, uncertainties are expressed through scenario analysis, using a limited number of physically realistic scenarios. The two scales are integrated by using the precautionary principle to merge the individual capture probability plumes corresponding to the different scenarios. The approach applies to both wellhead protection and the mitigation of contaminated aquifers, or in general, to groundwater management areas. An example relates to the WHPA for a supply well located in a complex glacial aquifer system in southwestern Ontario, where we focus on uncertainty due to the spatial distributions of recharge. While different recharge scenarios calibrate equally well to the same data, they result in different capture probability plumes. Using the precautionary approach, the different plumes are merged into two types of maps delineating groundwater management areas for either wellhead protection or aquifer mitigation. The study shows that calibrations may be non-unique, and that finding a “best” model on the basis of the calibration fit may not be possible.

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1. Introduction

Wellhead protection areas (WHPAs) serve the purpose of protecting the quantity and quality of water that flows into a well by means of restrictions imposed on land use activities within the WHPA. Most industrialized countries regulate WHPAs; for example, in the United States, the U.S. Environmental Protection Agency (US EPA, 1987, 1997) has developed guidelines for WHPA delineation, as has the Province of Ontario, Canada, through the Clean Water Act (Province of Ontario, 2004, 2006). WHPAs are usually delineated based on the estimated well capture zone, defined as the area from which the well draws its water, taking into account the travel times for water to reach the well screen.

Capture zones and WHPAs are normally delineated by means of mathematical modelling, which is subject to uncertainty due to many different factors. Hydraulic conductivity, heterogeneity, and boundary conditions are major sources of uncertainty, as is the recharge, both in terms of magnitude and spatial distribution. For capture zone delineation, uncertainties in the flow field become magnified in the delineation of the capture zone.

Uncertainty can be a barrier to the use of models, because decision makers may be reluctant to rely on uncertain model results (Brugnach et al., 2007; Poeter, 2007). Available methods to deal with uncertainty, such as the Monte Carlo approach, tend to be costly. As a result, uncertainty is not always taken into account in routine WHPA delineations. This paper presents a simple approach that should help to remove this barrier. First, uncertainty in capture zone delineation is considered at two scales – this helps in the conceptual understanding of uncertainty – and the two scales are then integrated. Second,
the approach is generalized to apply to both groundwater protection and the mitigation of groundwater contamination. The main goal is to improve the understanding of the causes and effects of uncertainties, and to make uncertainty analysis more transparent for practitioners and decision makers, hopefully leading to better modelling practices and more confidence in the use of models.

2. Background

A well-explored approach for addressing uncertainty in capture zone delineation is by means of stochastic methods, with contributions by, among others, Varljen and Shafer (1991), Franzetti and Guadagnini (1996), van Leeuwen et al. (1998), Camp and Outlaw (1998), Vassolo et al. (1998), Wheater et al. (2000), Kunstmann and Kinzelbach (2000), Feyen et al. (2001), and Stauffer et al. (2005). The general approach consists in expressing physical parameters (e.g. hydraulic conductivity) in terms of a statistical distribution, which is then used to generate capture zones expressed in terms of confidence levels or uncertainty bands.

Although stochastic methods provide a way to address uncertainty, there are some problems with this approach. Evers and Lerner (1998) pointed out that it is often impossible to characterize the statistical properties of model parameters using the available data. Also, as found by Refsgaard et al. (2005), stochastic methods in general only address uncertainty due to unknown parameter values, but usually neglect uncertainties in the model structure, including the overall problem geometry, the temporal and spatial discretization, the choice of processes being considered – hence, the governing equations to be solved – and different simplifying assumptions. A very similar argument was made by Poeter (2007).

As noted by Evers and Lerner (1998), for the stochastic approach to be applicable, the controlling parameters must be amenable to statistical description. A classical example is the work by Sudicky (1986), who sampled a sandy aquifer along a cross-section at the cm scale and developed the statistical parameters in terms of the variance of \( \log(K) \) and the correlation length. Assuming that the system is “homogeneously heterogeneous”, Sudicky applied the theory of Gelhar and Axness (1983) to derive effective macrodispersion coefficients that express the heterogeneity of the porous material. In a follow-up study, Frind et al. (1987) interpreted the evolution of macrodispersion as the cumulative effect of mass exchange between fast and slow streamtubes, thus providing a physical explanation for the macrodispersion theory. The heterogeneity of the material is an expression of uncertainty at the local scale of the sampling. Frind et al. (2002) applied the macrodispersion approach to delineate well capture zones in terms of capture probability, and in a different paper, Frind et al. (2006) used the same approach to develop the well vulnerability concept for estimating the impact of a contaminant source on a supply well. The fundamental theory underlying these two concepts was analyzed by Enzenhoefler et al. (2011), who used a conditional Monte Carlo simulation based on Bayes’ Theorem in discussing the relationship between the macrodispersion and stochastic (Monte Carlo) approaches, recommending the Monte Carlo approach for the well vulnerability problem.

Non-stochastic approaches have also been explored by some authors. For example, Esling et al. (2008) proposed a systematic sensitivity analysis using different recharge to hydraulic conductivity ratios. Evers and Lerner (1998) used alternative flow calibrations and backward particle tracking to define protection zones. West et al. (2011) proposed the delineation of wellhead protection areas using alternative flow scenarios associated with different weights based on technical judgement. Poeter (2007) suggested addressing predictive uncertainty by means of a reasonable set of alternative conceptual models, using multi-model averaging. Noting that geostatistical approaches are often considered first, she explained that “to capture the full conceptual uncertainty, one must look at broader variations of the configuration of geologic units, as well as alternative initial conditions, boundary conditions, processes, scenarios, dimensionality, and perhaps even alternative algorithms”.

Pappenberger and Beven (2006) argued that uncertainty analysis is still not a common practice in many modelling exercises. Lack of available guidance for use in practical applications is pointed out as a major reason. According to these authors, what exists is a number of alternative approaches with different philosophical frameworks, all of which are more or less appropriate, depending on the problem at hand. Although the authors made this argument for hydrology, hydraulics and water resources models in general, it can also be considered a fair portrayal of groundwater models applied to capture zone delineation.

3. An integrated approach for addressing uncertainty

For convenience, we consider a system of two spatial scales, local and global, each with its own type of uncertainty. Local-scale uncertainty is defined as the uncertainty generated by heterogeneities within a hydrogeological unit, of the type investigated by Sudicky (1986). Local-scale uncertainty can be addressed by stochastic methods, or alternatively, it can be approximated on the basis of macrodispersion theory (Gelhar and Axness, 1983) by applying a backward transport model to generate a capture probability distribution (Frid et al., 2002; Neupauer and Wilson, 1999). The macrodispersion approximation is valid if the scale of the hydrogeological unit is much larger than the scale of the local heterogeneities within the unit.

Global-scale uncertainty (where “global” refers to the model domain) incorporates a variety of other sources of uncertainty as discussed by Poeter (2007). These include the shape of the aquifer and aquitard units, the hydraulic connections between aquifer units (i.e. windows), the boundary conditions, the selection of processes to be considered and how they are represented (i.e. governing equations and modelling codes), uncertainties in the conceptual model, as well as the spatial and temporal discretizations. Sources of global-scale uncertainties are generally less amenable to stochastic treatment because often they cannot be described by parameters or parameter distributions. This type of uncertainty can be addressed by scenario analysis involving multiple model representations of the natural system (Poeter, 2007).

The concept of multi-model analysis may appear controversial within the context of conventional modelling practice, which aims to identify the “best” model among possible alternatives. Indeed, for many straight-forward situations, a best model can usually be defined without difficulty. On the
other hand, in more complex situations, it may not be possible
to unambiguously define the one “best” or “right” model—only
a number of possible candidates. In such cases, the question is
what to do with these alternatives.

Thus the scenario analysis leads to the problem of combining
a multitude of model predictions in a meaningful way for
decision-making. Statistical methods for ranking and averaging
multiple model predictions in numerical groundwater models
were developed and applied by Burnham and Anderson (2002),
Neuman (2003), Ye et al. (2004), Poeter and Anderson (2005),
Poeter and Hill (2007), Ye et al. (2008) and Singh et al. (2010).
Another way to combine different model predictions is by means
of the precautionary approach. This approach is well known to
policy makers and regulators, and is usually applied to make
decisions under uncertainty in situations where there is a
potential risk to the public or the environment and a conserva-
tive (i.e. risk-averse) stance is justified.

We propose a three-part approach to address uncertainty in
capture zone delineation: (1) express local-scale uncertainty
in terms of macrodispersion and apply backward transport
to generate a capture probability distribution; (2) express global-
scale uncertainty by using a reasonable number of alternative
scenarios or conceptual models of the real system; and (3) use
the precautionary approach to combine the multiple scenarios
into a capture zone. By expressing the result of each scenario
run in terms of a probabilistic distribution and combining these
distributions, the two uncertainty scales are effectively inte-
grated. At this stage, two types of groundwater management
areas can be defined, depending on whether the underlying
objective is protection of the groundwater resource or mitigation
of existing contamination. The components comprising the
proposed approach are explained in more detail in the following.

3.1. Local-scale uncertainty: Capture probability

At the scale of the individual stratigraphic unit, the
porous material may be considered homogeneously het-
erogeneous (i.e. statistically stationary) (Sudicky, 1986). The
macrodispersion approach (Gelhar and Axness, 1983) applies,
and a well capture zone can be expressed in terms of capture
probability (Frind et al., 2002; Neupauer and Wilson, 1999).
Frind et al. (2002) compared the capture probability approach to
the standard particle tracking approach, which is currently the
industry standard for delineating well capture zones, showing
that capture probability produces more realistic capture zones
than particle tracking, with less need for subjective judgement.

To implement the capture probability approach, a standard
advective-dispersive transport model in backward mode (with
the sign on the advective term reversed) is applied to solve for
capture probability with respect to the well. The simulation
process can be compared to the tracking of particles upgradient
from a well, except that a dispersion term is added to represent
local-scale uncertainty. The transport boundary condition at
the well is a specified capture probability of 1.0. The result is a
plume of capture probability extending upgradient from the
well toward the ground surface, similar to a contaminant
plume extending downgradient, obtained when solving the
equation in the forward mode.

Use of the advection-dispersion equation for this purpose
is valid, because the equation describes the physical process
of advection due to a flow field, combined with dispersive
spreading through the porous medium, and it can be applied
to any quantity subjected to this process (e.g. solute mass,
age, etc.). Here we apply this equation to a fictitious quantity
that has a value of 1.0 at the well screen and tends to zero
infinitely away from the well, and we choose to interpret the
result as capture probability.

The capture probability concept represents a refinement of
the conventional approach for delineating a capture zone,
which is based on a line drawn on a map dividing an area into
“inside” (capture, or 100% capture probability) and “outside”
(no capture, or 0% capture probability) segments. The conven-
tional approach can cause problems because a property owner
just inside the line may face land use restrictions that his/her
neighbour just outside the line would not encounter. Concept-
ually, a more realistic way to assess the risk of contamination
would be to assign a capture probability of less than 100% to the
area just inside the line, and more than 0% to the area just
outside the line. This means that, for example, we may judge
the chances of well contamination due to a source at some point
inside the line at 75% (capture probability P = 0.75). The
capture probability concept formalizes this straightforward
approach, producing a continuous probability spectrum from
100% (at the well itself) to 0% (very far from the well).

This concept could replace the traditional “line-on-the-map”
concept. However, if required for planning purposes, a line on the
map can still be recovered easily from the probability distribu-
tion by choosing a capture probability contour appropriate for
the problem at hand. Molson and Frind (2012) suggested the 0.5
contour on the basis of life expectancy considerations. Another
option is to select a contour on the basis of mass balance between
recharge and pumping (Frind et al., 2002).

It should be noted that capture probability will not predict
the actual impact on a well. Capture probability simply puts
a number on the risk level. It means that, for example, a
contaminant source on the 0.75 probability contour will pose a
higher risk of impacting the well than a source on the 0.5
contour. To determine the actual impact of a specific contami-
nant source on a well, forward solute transport runs or the well
vulnerability method (Enzenhoefer et al., 2011; Frind et al.,
2006) can be used. The well vulnerability method provides the
maximum concentrations to be expected at the well, plus the
arrival and exposure times, due to any source of contamination
within the capture zone. This method uses the same advective-
dispersive transport equation as the capture probability method,
except that instead of the specified value of 1.0 at the well, a
pulse is applied at either the contaminant source or the well;
the resulting breakthrough curve then provides the desired
information.

3.2. Global-scale uncertainty: Scenario analysis

Capture probability, as defined above, expresses only the
local-scale component of uncertainty. The global-scale compo-
nent of uncertainty can be assessed by scenario analysis
involving a limited number of realistic conceptual model
configurations and boundary conditions (Evers and Lerner,
1998; Poeter, 2007; West et al., 2011; also others). These
scenarios can be seen as different realizations or attempts to
represent a complex system, where perturbations are based
on physical rather than statistical principles and follow no
particular pattern. Different scenarios can be created by
developing alternative conceptual models, applying different boundary conditions, changing the geometry and/or the hydraulic characteristics of hydrostratigraphic units, using different grid types or discretizations, or by using different codes.

By allowing the incorporation of alternative model structures, the robustness of model predictions can be enhanced (Refsgaard et al., 2007). The only requirement for a model scenario to be considered is that it should be a valid representation of reality based on a realistic conceptual model with reasonable parameter distributions and boundary conditions, and it should be solved using an accepted, verifiable numerical method. Because the differences between scenarios may be substantial, each scenario must be calibrated against the original field data. A successful calibration, however, is only a necessary, but not a sufficient condition for validity (Oreskes et al., 1994). As will be shown below, different scenarios can calibrate equally well to the same data.

### 3.3. Integrating multiple scenarios: The precautionary approach

If there is more than one valid representation for a given situation, as is the case for most practical applications, it is impossible to objectively choose which is “the best” representation (Carrera and Neuman, 1986). However, simply presenting a collection of alternative capture zones arising from different scenarios/models would not be very useful in the decision-making process, and it would overload decision makers with information. Also, it would not address the critical problem of how to delineate capture zones under uncertain conditions. In order to facilitate the decision-making process, alternative capture zones must be combined or integrated in a systematic and transparent way. West et al. (2011), for example, used technical judgement in the weighing of different scenarios to arrive at a final capture zone. A logical choice for combining or integrating the results from alternative model scenarios, which we will use here, is the precautionary approach. The precautionary approach follows the intent of the Precautionary Principle as defined formally in the Wingspread statement (Raffensperger and Tickner, 1999): “When an activity raises threats of harm to human health or the environment, precautionary measures should be taken even if some cause and effect relationships are not fully established scientifically”. The Precautionary Principle is often used in a regulatory context, and it generally applies to decision-making under uncertain conditions without necessarily quantifying the uncertainty. For example, one of the guiding principles of source protection in the Province of Ontario is that “Source protection plans must be based on risk management, when risks can be estimated, and the precautionary principle when risks cannot be estimated” (Province of Ontario, 2004).

The precautionary approach for the delineation of well capture zones, or more generally, groundwater management zones, can be considered as appropriate because an independent validation of a well capture zone is rarely possible. Tracer tests would in most situations simply take too long, monitoring would carry its own uncertainties, and furthermore, the introduction of tracers into a water supply aquifer may be undesirable. Therefore, the precautionary approach should be a defensible option in practical situations.

### 3.4. Protection versus mitigation

In the context of wellhead protection, the “precautionary measure” pertains to the inclusion or exclusion of a given area in a WHPA. This decision depends on the purpose of the decision-making exercise, where we distinguish between two objectives: (a) protection of groundwater resources, and (b) mitigation of groundwater contamination.

For example, let’s imagine that there is doubt whether a certain point \((x,y)\) at ground surface is inside or outside the capture zone of a given well. If the objective is to define protection zones to keep contaminants from reaching the well (e.g. choosing the location for a new landfill), then the “precautionary measure” is to assume that point \((x,y)\) is inside the capture zone. This measure preferentially overestimates the extent of the capture zone and decreases the chance of placing a potentially hazardous activity inside the true capture zone of the well.

Alternatively, the objective may be to define capture zones for the hydraulic containment of contaminated areas (i.e. hydraulic barriers), or to prioritize sites for the implementation of Beneficial Management Practices or BMPs (Wassenaar et al., 2006) in order to enhance water quality at the well. Now the “precautionary measure”, in case of doubt, is to assume the given area falls outside the capture zone. This preferentially underestimates the extent of the capture zone and increases the chances that flow through the designated BMP areas will ultimately be captured by the well, benefiting the mitigation objective.

Fig. 1, adapted from Evers and Lerner (1998), graphically illustrates the concept. The left part of the figure shows possible capture zones generated by a number of alternative model scenarios; to the right appear the resulting management areas corresponding to either a protection-based objective or a mitigation-based objective. For a protection decision, the precautionary approach would consider the union of all alternative capture zones, while for a mitigation decision it would consider the intersection of alternative capture zones. Evers and Lerner (1998) called these areas the “zone of uncertainty” and the “zone of confidence”, respectively. Because the extent of the area subject to management measures has economic as well as environmental and social implications, professional judgement should be exercised in the creation and selection of scenarios, as well as in the application of the precautionary principle.

### 3.5. Mathematical formulation

The proposed integrated approach can be implemented mathematically through two simple equations. These equations combine capture probability estimations (i.e. local-scale uncertainty) from multiple scenarios (i.e. global-scale uncertainty), in a risk-averse manner (i.e. precautionary approach). For protection decisions, the equation is:

\[
P_{\text{PROT}}(x, y, t_C) = \max \{P_1(x, y, \forall z, t_C), P_2(x, y, \forall z, t_C), \ldots, P_N(x, y, \forall z, t_C)\} \tag{1}
\]

where \(P_{\text{PROT}}(x, y, t_C)\) is the maximum probability, from all scenarios, that a particle at a given point \((x, y)\) will be
captured within a time period not greater than \( t_c \). For example, a \( P_{\text{ROI}}(x,y,80) = 0.5 \) means that, for the position \((x,y)\) on this contour, all simulations estimate that the groundwater infiltrated at point \((x,y)\) has a probability of capture of 50% or lower, within 80 years. The resulting protection map combines the maximum estimated probabilities throughout the vertical extent of the model domain, from the bottom to ground surface. This is also a conservative assumption, assuming that there may be vertical preferential flow paths.

For mitigation decisions, the equation to be used is:

\[
P_{\text{MIT}}(x,y,t_c) = \min[P_1(x,y,z_{GS}, t_c), P_2(x,y,z_{GS}, t_c), \ldots , P_N(x,y,z_{GS}, t_c)]
\]  

(2)

where \( P_{\text{MIT}}(x,y,t_c) \) is the minimum probability, from all scenarios, that a particle at a given point \((x,y)\) at ground surface \((z_{GS})\) will be captured within a time period not greater than \( t_c \). For example, \( P_{\text{MIT}}(x,y,80) = 0.5 \) means that, for the position \((x,y)\), all simulations estimate a probability of capture by the well of 50% or higher, within 80 years. Overestimating the probability of capture is not desirable in this case, so the values at ground surface are taken into account.

In this way, the information from all scenarios is merged into two types of maps for guiding management decisions: one for protection and one for mitigation. This reduces information overload for decision makers, increases efficiency, and makes modelling results more transparent and understandable to stakeholders, as suggested by Brugnach et al. (2007).

The methodology is based on the assumption that erring on the side of caution is desirable, and accordingly, it mathematically expresses the postulate that when making decisions subject to doubt, consider the worst-case situation amongst the available alternative interpretations of the natural system. The rationale behind this postulate, and hence this methodology, cannot be proven or disproven using physical field data. It is merely the mathematical translation of a precautionary (risk-averse) approach to combining alternative representations of well capture zones to support groundwater management decisions. Using control theory terminology, this approach attempts to be “fail-safe”, defined as “a system which fails to a state that is considered safe in the particular context” (Blanke et al., 2001).

4. Example application: Water supply well, Waterloo Moraine

The approach outlined above was applied to delineate the protection and mitigation capture zones for one of the water supply wells (average pumping rate = 6756 m³/day) that are part of a system of well fields operated by the Regional Municipality of Waterloo, Ontario, Canada. The well is located within the Waterloo Moraine (Fig. 2), a complex glacial aquifer system that is of importance as a source of water for the local community of over half a million people. The health of the local aquatic ecosystem also depends on the groundwater. The Waterloo Moraine has been the focus of many field and modelling studies (Bester et al., 2006; Callow, 1996; CH2M-HILL and S.S. Papadopoulos and Associates, 2003; Frind et al., 2002, 2006; Martin, 1994; Martin and Frind, 1998; Rahman et al., 2011).

For the sustainability of groundwater resources, recharge plays a key role and its estimation is usually associated with significant uncertainty, even when averaged temporally and spatially (Stauffer et al., 2005). Although this approach can be applied to many different sources of uncertainty, we focus here on the uncertainty in the spatial distribution of recharge.

4.1. Waterloo Moraine model

The groundwater flow model that underlies our study is based on the original Waterloo Moraine model by Martin and Frind (1998). The conceptual model is bounded by major water courses (Grand River, Nith River and Conestogo River), and covers an area of 740 km² (Fig. 2). The model is based on the assumption that at the river boundaries, all water discharges into the river, and that regional flow crossing beneath the river is negligible. This assumption provides a no-flow model boundary around the periphery of the model. Major water courses on the boundary and in the interior of the domain are represented by specified heads. Vertically, the model consists of 8 hydrostratigraphic layers. The original groundwater flow simulations were performed using WATFLOW (Molson et al., 2002), a 3D finite-element groundwater flow model. This code also contains a built-in automatic calibration routine (Beckers and Frind, 2001), which facilitates the calibration of multiple flow scenarios.

The present study uses the original Waterloo Moraine model with its original boundary conditions for flow, but focuses on the rectangular area shown in Fig. 2 for detailed capture zone simulations. Within this smaller study area, the hydraulic conductivity distribution of Martin and Frind (1998) was updated using new data provided by the Regional Municipality of Waterloo. The model discretization was refined within the smaller area, with 29 elemental layers, giving a total of ~1,300,000 nodes and ~2,500,000 elements.

4.2. Alternative recharge scenarios

To assess uncertainty in the spatial distribution of recharge, three alternative recharge distributions generated by different codes were used: (1) HydroGeoSphere (Therrien et al., 2005) as
applied by Jones et al. (2009), (2) GAWSER (Schroeter and Associates, 1996) in association with MODFLOW (Harbaugh et al., 2000), as applied by CH2M-HILL and S.S. Papadopulos and Associates (2003), and (3) WATFLOW. Each of these three models is based on valid theories, and, although different, the corresponding recharge distributions can all be considered as physically realistic. All are approximations because they are based on limited data.

HydroGeoSphere (HGS) is a 3D fully-integrated surface and variably-saturated subsurface flow code, including solute and heat transport. HGS adopts a rigorous approach to representing the interaction between different components of the hydrological cycle. Surface water is represented using the diffusion-wave approximation of the Saint Venant equation (Govindaraju et al., 1988). Unsaturated flow is simulated using the Richards equation with the van Genuchten parameterization (van Genuchten, 1980) to estimate saturation (S) and hydraulic conductivity (K) as a function of pressure head. The recharge distribution was taken from the work of Jones et al. (2009).

GAWSER is a storm-event surface water model, which was coupled to the finite-difference groundwater model MODFLOW. Unsaturated flow is not represented. This recharge distribution was taken directly from an existing study (CH2M-HILL and S.S. Papadopulos and Associates, 2003).

In WATFLOW, the recharge distribution is estimated using the recharge spreading layer (RSL), a virtual layer of porous material placed on top of the ground surface, emulating interflow in the surficial layer (Fig. 3). Darcian flow in the RSL is assumed. An average recharge value is specified on top of this layer; this recharge is redistributed within the RSL to avoid mounding on low-K materials. Thus the hydraulic conductivity of the recharge spreading layer controls to what extent recharge is spatially distributed. Accordingly, the hydraulic conductivity of the RSL becomes a calibration parameter.

The recharge distributions produced by these three different models are presented in Fig. 4 for HGS, GAWSER/MODFLOW and WATFLOW, respectively. As the original recharge distributions for HGS and GAWSER/MODFLOW did not cover the whole area of the model domain used for the simulations, an average recharge of 250 mm/year was assigned where recharge estimations were not available. The supply well which will be the focus of the capture zone delineation is shown in the figure.

In each of the three models, the recharge (i.e. the actual downward flux that infiltrates at ground surface and eventually
reaches the water table) is an internally calculated quantity that depends on the processes built into the model. Since these processes vary for the three models, the average recharge within the model area (calculated by averaging the downward fluxes) differs somewhat (212 mm/year for HGS; 233 mm/year for GAWSER/MODFLOW; and 255 mm/year for WATFLOW), but the differences are small enough to allow the recharge magnitude to be discounted as a major control. Accordingly, the spatial variation of recharge is taken to be the controlling parameter.

For HGS, the generated recharge distribution (Fig. 4a) covers approximately the southeast quadrant of the study area. The blue areas indicate a gaining stream. Contrary to expectations, the three gravel pits within the area do not affect the recharge distribution produced by HGS. The GAWSER/MODFLOW recharge distribution (Fig. 4b) covers the southern part of the study area. The GAWSER/MODFLOW recharge differs significantly from that generated by HGS, on account of the very different mechanism built into this model. Recharge in this model is controlled by surface soil type and depression-focused infiltration (i.e. closed-basin areas in which runoff accumulates); these mechanisms result in a high spatial variability of recharge with numerous areas of either high or low values. In particular (see Fig. 4b), there is a large area of low recharge near the centre of the study area, flanked to the south by areas of high recharge. WATFLOW covers the entire study area (Fig. 4c), controlling recharge by means of its recharge spreading layer (Fig. 3), which simulates interflow. For the WATFLOW simulation, a recharge value of 600 mm/year was assigned a priori to the gravel pits. This value was obtained during calibration, using an expert estimate (P. Martin, personal communication, 2009) as a starting value. The result is a recharge distribution which is intermediate between those of HGS and GAWSER/MODFLOW. A consequence of the differing recharge distributions for the three scenarios is that the stream segments that are gaining/losing are not the same between the models.

4.3. Steady-state flow calibration

Three alternative steady-state flow models (one for each recharge scenario) were calibrated to match observed heads in 42 wells. To achieve calibration, the hydraulic conductivity for each hydrostratigraphic unit was allowed to vary within one order of magnitude. This range is comparable with the error bounds for field estimation methods commonly used at this scale (Alexander et al., 2011). All three flow models were calibrated starting from the same initial hydraulic conductivity distribution. Therefore, differences in the calibrated hydraulic conductivity field are commensurate with changes in recharge, as the target calibration data set used for the three models is the same.
This process resulted in comparable calibration fits for all three scenarios, as shown in Fig. 5. The average error ranges between −2.5 m (GAWSER/MODFLOW) and 2.4 m (HGS), while the average absolute error ranges between 4.0 m (GAWSER/MODFLOW) and 2.4 m (WATFLOW). This error compares to a range in head of about 80m over the model domain. As an independent verification, an observed baseflow value for a creek located within the studied area was found to be comparable to calculated discharge estimations for all three scenarios. Because of the approximate nature of the data, it would be pointless to try to select a “best” model from the three conceptual model scenarios. Thus the conclusion from the calibration is that the three models are all acceptable, but non-unique.

4.4. Conventional approach to capture zone delineation: Particle tracking

The capture zone delineation focuses on the primary supply well identified in Figs 4 and 6. Fig. 6 also shows additional municipal wells which are not directly considered for capture zone delineation, but which strongly influence the flow field. To delineate the primary well capture zone for each of the three scenarios, the conventional backward particle tracking approach was first applied to the three recharge scenarios, using the particle tracking routine WATRAC (Frind and Molson, 2004). Particles were placed around a circle at the well and allowed to travel in the upgradient direction from the well within the 3D flow field, until they emerged at ground surface. The results are shown in Fig. 6. The tracks represent advective travel only, with no uncertainty due to local-scale heterogeneities taken into account.

The three sets of particle tracks extend generally from the primary supply well toward the northwest, and their shape and orientation is influenced by the other wells in the well field. A portion common to all three scenarios extends first to the north, and then curves to the west. Beyond this common portion, HGS (Fig. 6a) has a leg extending to the northwest, while GAWSER/MODFLOW (Fig. 6b) has a similar northwest tending leg, but displaced toward the east. WATFLOW (Fig. 6c) has no extension beyond the common portion.

Delineating a capture zone from the above particle tracking results would clearly require some judgement. If local-scale uncertainty is to be addressed, one way to accomplish this is by means of a standard Monte Carlo analysis, creating a sufficiently large number of realizations for each of the three scenarios, and applying particle tracking to each realization. Alternatively, local-scale uncertainty can also be accounted for by means of the capture probability method, which we demonstrate in the following.

4.5. Capture probability and scenario analysis

To apply the capture probability method, an advective-dispersive transport model in backward mode is run for each of the three calibrated scenarios. The transport code WTC (Molson and Frind, 2005) was used for this purpose. Dispersion coefficients of 20 m, 5 m, and 0.02 m were chosen for longitudinal, horizontal transverse and vertical transverse directions, respectively, as in earlier studies of this system (Frind et al., 2002). The model was run to quasi-steady-state conditions, which was approached at 180 years. From these 3D capture probability distributions, two sets of maps were extracted: (1) the maximum capture probability over the aquifer depth for the three recharge scenarios (Fig. 7), obtained from the 3D model output by selecting, for each point (x,y) in the horizontal plane, the maximum value in the vertical direction, and (2) the capture probability at ground surface for the three recharge scenarios (Fig. 8), obtained by plotting the intersection of the 3D probability plume with the ground surface. For ease of interpretation, the 0.5 contour has been emphasized in all figures.

These figures show that, although the calibration leads to the same fit for each scenario, the capture probability plumes obtained differ significantly between scenarios. A major influence on the shape of the plumes is on account of the wells immediately to the northwest of the primary well, which produce indentations in the capture zone for the primary well. Another group of wells farther to the northwest, however, impacts mainly the HGS (Fig. 7a) and WATFLOW (Fig. 7c) plumes. For HGS, these wells cause the plume to split into two branches extending to the northwest, while for WATFLOW, only one branch extends to the northwest. For GAWSER/MODFLOW, the wells to the northwest seem to restrain mainly the higher probability values (>0.5) for the primary well, but not the lower values, resulting in a large plume extending to the northwest.

The capture probability plumes at ground surface (Fig. 8a, b, and c) show basically the same trends as Fig. 7, except that at the surface, the plumes are somewhat smaller and more irregular. This shows that the maximum extent of a capture zone occurs at depth, which supports the need for a 3D analysis.

The differences in the probability plumes for the different scenarios demonstrate the high sensitivity of capture probability with respect to recharge. In particular, the large size of the GAWSER/MODFLOW plume could be related to the large area of low recharge (Fig. 4b), which coincides with the centre of the probability plume (Fig. 7b) for this scenario. On the other hand, local features such as the stream or the gravel pits do not seem to have a significant effect on capture probability.

Fig. 5. Calibration plot for three different model scenarios with different recharge distributions (HydroGeoSphere, GAWSER/MODFLOW and WATFLOW).
In terms of a final capture zone, it should be kept in mind that the capture zone of most interest will be the combined capture zone for all supply wells. In this combined capture zone, the indentations seen in Figs. 6, 7, and 8 would not occur. Considering only one well out of a group of wells in the same well field, as we have done here, results in a sharp gradient in the individual probability functions, resulting in numerical dispersion. This problem is less likely to occur when all wells in the well field are investigated together.

A high capture zone sensitivity with respect to hydrogeologic parameters has also been observed in other studies, such as Piersol (2005) and Franke et al. (1998).

4.6. Groundwater management areas: Protection vs. mitigation

The two sets of maps in Figs. 7 and 8 can be used to generate two single maps delineating groundwater management areas under either the protection or the mitigation objective, using Eqs. (1) and (2). The process is schematically shown in Fig. 1. To generate the protection map for the primary supply well (Fig. 9), the maximum capture probabilities over all scenarios in Fig. 7 are chosen on a point-by-point basis. For the mitigation map for the same well (Fig. 10), the same point-by-point approach is taken, but now the minimum capture probability at ground surface over all scenarios in Fig. 8 is chosen. In both cases, these maps provide conservative predictions for each location based on the three selected scenarios and the type of decision to be made.

A comparison of Figs. 9 and 10 shows that the capture probability maps for protection and mitigation differ substantially for this well. While the management area for protection is about 5 km wide and extends nearly 20 km to the northwest from the well, the management area for effective mitigation is only about 1 km wide by 3 km long extending in the northerly direction. The difference in this case is primarily due to the uncertainty in the recharge distribution. If other uncertainties were to be considered, the distinction between the protection and mitigation maps would likely be even larger.

As a final question, we may ask whether a valid capture zone can be delineated by simply merging the particle tracks from the three scenarios. The result is given in Fig. 11, which shows the particle tracks from Fig. 6, with the 0.5 probability contour from Fig. 9 superimposed. As is evident from the figure, the 0.5 contour provides a reasonable envelope for the particle tracks. This demonstrates that particle tracks from different scenarios can be merged to provide a capture zone that takes global-scale uncertainty into account. In the present case, however, drawing the envelope without the benefit of the 0.5 contour would require considerable judgement. Thus the capture probability approach can be seen as being less subjective and more informative than particle tracking by itself.

5. Discussion: Some key points

This study has raised some key points that are highly relevant in the appreciation of uncertainty in modelling.

5.1. Scenario selection

Care should be taken that only scenarios that are physically realistic and representative are included. The analysis can be only as good as the technical judgement behind the formulation and selection of these scenarios. This is a limitation of any modelling endeavour, but since this approach uses a conservative stance, for every scenario that is added, the resulting groundwater management areas can only become
more conservative or remain the same. Therefore, the inclusion of one single inadequate scenario may render the final delineation excessively conservative.

Fig. 7. Maximum capture probability over aquifer depth using recharge distributions from (a) HydroGeoSphere, (b) GAWSER/MODFLOW, and (c) WATFLOW. The 0.5 contour has been emphasized.

Fig. 8. Capture probability at ground surface using recharge distributions from (a) HydroGeoSphere, (b) GAWSER/MODFLOW, and (c) WATFLOW. The 0.5 contour has been emphasized.

5.2. Dealing with expert subjectivity

Due to the subjectivity that is typically inherent in expert judgment, different interpretations may be expected from different experts working on the same problem (e.g. Beven,
The proposed approach provides a framework for incorporating the uncertainty derived from different experts by combining the results in a conservative manner. This eliminates the difficult (or impossible) task of unquestionably selecting the “best” or “right” model among a set of alternative valid representations. Because the problem of choosing the “right” model is eliminated, this approach should reduce the potential for litigation.

5.3. “Safest decision” vs. “Optimum decision”

The precautionary nature of this method leads naturally to more conservative and safer decisions than a decision based on a single scenario. But safety has a price. For protection applications, this method can lead to the imposition of restrictions in areas that may not significantly impact the well, while for mitigation applications, it may exclude areas that could possibly contribute to the well. The approach does not lead to “optimum decisions”, as some statistical methods do. Instead, it aims to make the “safest decision” based on the available interpretations of the real system, in a transparent and pragmatic manner. Practitioners should keep in mind that, even with this precautionary stance, it is impossible to exhaust all relevant possible combinations of valid models. Therefore, the protection and mitigation maps do not necessarily represent the absolute worst-case predictions that can possibly be made, as there is always a possibility that an important model interpretation could have been left out of the analysis (Refsgaard et al., 2007).

5.4. Cost considerations

The proposed approach does not require more data than the conventional approach; the same dataset that is used to create one scenario can be also used to generate alternative scenarios. However, multi-model analysis does require more time than single-model analysis. The additional cost will depend on whether alternative scenarios are based on different models or on modifying parameters within the same model. In any case, modelling costs are usually a small percentage of overall costs of source water protection studies.

5.5. Field data vs. modelling

It is important to keep in mind that modelling can never be a substitute for field data. The proposed method expresses uncertainty, but does not reduce it. To reduce uncertainty, additional data should be collected and incorporated in the model. For example, direct field estimations of recharge would constrain the distribution of this parameter in the model and consequently reduce model uncertainty.

6. Conclusions

We have attempted to provide some new insights into the problem of uncertainty in capture zone delineation for complex systems that are not readily amenable to stochastic analysis. For these systems, we propose that uncertainty be considered at two scales. At the local scale of the stratigraphic unit, the porous material may be considered heterogeneously homogeneous,
and the resulting uncertainty can be represented by using the macrodispersion concept, leading to a capture probability distribution. At the larger global scale, where uncertainty is due to a variety of causes including structural uncertainty and uncertainty in the boundary conditions, uncertainty can be addressed by means of systematic scenario analysis over a number of different but physically plausible scenarios, with each being calibrated individually against field data.

Results from multiple scenarios can be integrated using the precautionary approach to delineate groundwater management areas under either of the two objectives: (1) the protection of groundwater sources, and (2) the mitigation of contaminated areas by means of remedial measures. For the first objective, the precautionary approach leads to a conservative capture zone based on the combination of all areas that might contribute to capture. For the second objective, it leads to an equally conservative capture zone based on the selection of all areas with high probability of capture that are most likely to contribute to flow to a given well. Both objectives can be covered within the same investigation.

We have shown that the spatial distribution of recharge can have a controlling impact on capture zone delineation, and thus be a major source of uncertainty. The wide range of recharge values generated by different models stresses the importance of independent recharge estimation using field methods to constrain this range, and thus to reduce uncertainty.

We have also shown that equally acceptable calibration fits can be obtained from different recharge distributions, thus illustrating non-uniqueness. In current practice, modellers tend to choose the “best” model on the basis of the calibration outcome, where the “best” model or scenario is taken to be the one with the best calibration fit to observed data, and other reasonable model representations may be discarded. Our work shows that this can lead to serious underestimation of a capture zone. By including all acceptable or valid models in the analysis, large-scale uncertainty can be accounted for by means of the precautionary approach.

Although this study has expanded the range of uncertainties that are commonly dealt with, we hope that it has also produced more clarity into its effects. Because uncertainty will remain elusive, model users and decision makers need to be aware of the causes of uncertainty and alert in detecting its effects. This means that technical judgement will always play a role throughout the process, particularly in the selection of scenarios. It also means that in examining model results obtained under uncertainty, the first question should always be: Do the results make sense? Unfortunately, in a high-pressure consulting environment, there may not always be sufficient opportunity to ask this question.

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