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SOURCE WATER PROTECTION BASED ON UNCERTAINTY OF DYNAMIC CAPTURE ZONES USING MIKE SHE

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Abstract: Well head protection areas (WHPAs) are a common planning tool for reducing the risk of contamination to drinking water supply wells. Typical WHPA delineation involves steady-state groundwater flow modeling with deterministic backward particle tracking. However, WHPAs based solely on steady-state groundwater models ignore or simplify processes outside of the saturated groundwater zone and neglect important dynamic and transient effects. The comprehensive watershed-modelling tool, MIKE SHE, can treat many water management issues in an integrated fashion, at a wide range of spatial and temporal scales. MIKE SHE was recently used in Denmark to evaluate the uncertainty associated with WHPA delineation, which is ignored in traditional, deterministic WHPAs delineation. A sensitivity analysis was done to determine the 16 most sensitive parameters. Then, using MIKE SHE's automatic calibration and Monte Carlo utilities, nearly 1000 simulations were distributed across a local intranet to take advantage of idle computer resources at night. The results of this analysis were used to determine the areas that most likely contribute water to the wells and, thus, optimize planning restrictions for stakeholders.

Key Words: MIKE SHE, integrated modelling, Monte Carlo, capture zones, particle tracking

INTRODUCTION

The water resources around the world are under increasing pressure due to rapid population and economic growth, aggravated by a lack of coordinated management and governance (UNESCO, 2003). Water shortage, deteriorating water quality and flood impacts are among the most urgent problems that need attention. However, the problems are seldom isolated and their solution requires a holistic approach to water management that must address different, often conflicting, demands for water. Nor does water movement follow political boundaries, which creates conflicts and further fragments management activities, (Jensen et al., 2002). Thus, increasingly, water resources are being managed on a watershed basis, while addressing problems at the local scale.

Changing to a watershed-based water management system challenges not only our management structures, but it also requires new and more sophisticated tools. Traditional groundwater and surface water models were not designed to answer questions related to conjunctive use of groundwater and surface water, water quality impacts of surface water on groundwater, impact of land-use changes and urban development on water resources, and floodplain and wetland management. Instead, fully integrated hydrologic models of the watershed behaviour are required. These models must not only describe the water flow processes in an integrated fashion, but they must also be able to describe the movement of sediment, chemicals, nutrients, and water-borne organisms and their role in watershed habitats and ecology.

In this paper, we look at the comprehensive watershed-modelling tool MIKE SHE and how it was used to determine the uncertainty associated with dynamic capture zones for well head protection. The first section provides a general background of the MIKE SHE model and reviews the hydrologic processes included in the MIKE SHE modeling framework. Next we look at the methods available in MIKE SHE for dynamic capture zone analysis. Finally, we provide a summary of a project, where MIKE SHE was used to determine the uncertainty associated with dynamic capture zones for well head protection.

HYDROLOGIC MODELING AND MIKE SHE

In the hydrological cycle, water evaporates from the oceans, lakes and rivers, from the soil and is transpired by plants. This water vapour is transported in the atmosphere and falls back to the earth as rain and snow. It infiltrates to the groundwater and discharges to streams and rivers as base flow. It also runs off directly to streams and rivers that flow back to the ocean. The hydrologic cycle is a closed loop and our interventions do not remove water; rather they affect the movement and transfer of water within the hydrologic cycle.

In 1969, Freeze and Harlan (Freeze and Harlan, 1969) proposed a blueprint for modelling the hydrologic cycle. In this original blueprint, different flow processes were described by their governing partial differential equations. The equations used in the blueprint were known to represent the physical processes at the appropriate scales in the different parts of the hydrological cycle. From 1977 onwards, a consortium of three European organizations[1] developed, and extensively applied, the Système Hydrologique Européen (SHE) based on the blueprint of Freeze and Harlan (Abbott et al., 1986a & b). From this work emerged the integrated hydrological modeling system MIKE SHE.

Since the mid-1980's, MIKE SHE has been further developed and extended by DHI Water & Environment. Today, MIKE SHE is an advanced, flexible framework for hydrologic modelling. It includes a full suite of pre- and post-processing tools, plus a flexible mix of advanced and simple solution techniques for each of the hydrologic processes. MIKE SHE covers the major processes in the hydrologic cycle and includes process models for evapotranspiration, overland flow, unsaturated flow, groundwater flow, and channel flow. Each of these processes can be represented at different levels of spatial distribution and complexity, according to the goals of the modelling study, the availability of field data and the modeller's choices, (Butts et al. 2004). The MIKE SHE user interface allows the user to intuitively build the model description based on the user's conceptual model of the watershed. The model data is specified in a variety of formats independent of the model domain and grid, including native GIS formats. At run time, the spatial data is mapped onto the numerical grid, which makes it easy to modify the spatial discretisation of the model as needed. Finally, MIKE SHE also includes modules for water quality, irrigation management, full water balance accounting, particle tracking and parameter estimation.

MIKE SHE uses MIKE 11 (Havnø et al. 1995) to simulate channel flow. MIKE 11 includes comprehensive facilities for modeling channel networks, lakes and reservoirs, as well as river structures, such as gates, sluices, and weirs. In many highly managed river systems, accurate representation of the river structures and their operation rules is essential. In a similar manner, MIKE SHE is also linked to the MOUSE sewer model (e.g. Mark et al, 2004), which can be used to simulate the interaction between urban storm water and sanitary sewer networks and groundwater. MIKE SHE is applicable at spatial scales ranging from a single soil profile, for evaluating crop water requirements, to large regions including several river catchments, such as the 80,000 km^2 Senegal Basin (e.g. Andersen et al., 2001). MIKE SHE has proven valuable in hundreds of research and consultancy projects covering a wide range of climatological and hydrological regimes. Graham and Butts (2005) includes a large number of references to easily accessible journal articles, where MIKE SHE has been used.

The need for fully integrated surface and groundwater models, like MIKE SHE, has been highlighted by several recent studies (e.g. Camp Dresser & McKee Inc., 2001; Kaiser-Hill, 2001; West Consultants Inc. et al., 2001; Kimley-Horn & Assoc. Inc. et al., 2002; Middlemis, 2004, which can all be downloaded from the MIKE SHE web site). These studies compare and contrast available integrated groundwater/surface water codes. They also show that few codes exist that have been designed and developed to fully integrate surface water and groundwater. Further, few of these have been applied outside of the academic community (Kaiser-Hill, 2001).

Process-based hydrologic modeling

MIKE SHE, in its original formulation, could be characterized as a deterministic, physics-based, distributed model code. It was developed as a fully integrated alternative to the more traditional lumped, conceptual rainfall-runoff models. A physics-based code is one that solves the partial differential equations describing mass flow and momentum transfer. The parameters in these equations can be obtained from measurements and used in the model. For example, the St. Venant equations (open channel flow) and the Darcy equation (saturated flow in porous media) are physics-based equations. There are, however, important limitations to the applicability of such physics-based models. For example,

- it is widely recognized that such models require a significant amount of data and the cost of data acquisition may be high;
- the relative complexity of the physics-based solution requires substantial execution time;
- the relative complexity may lead to over-parameterized descriptions for simple applications; and
- a physics-based model attempts to represent flow processes at the grid scale with mathematical descriptions that, at best, are valid for small-scale experimental conditions.

In most watershed problems, one or two hydrologic processes dominate the watershed behaviour. For example, flood forecasting is dominated by river flows and surface runoff, while wetland restoration

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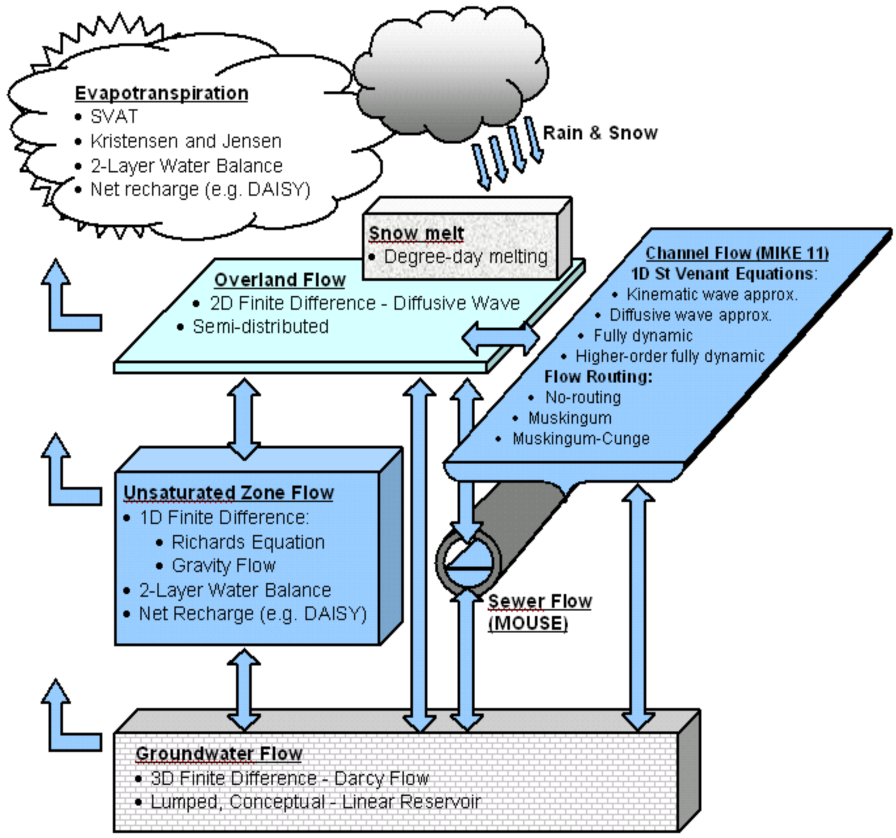

Figure 1 Schematic view of the processes in MIKE SHE, including the available numeric engines for each process. The arrows show the available exchange pathways for water between the process models. *From Graham and Butts (2005)*

depends mostly on saturated groundwater flow and overland flow. Thus, a complete, physics-based flow description for all processes in one model is rarely necessary. A sensible way forward is to use physics-based flow descriptions for those processes that are important in the particular context, and simpler, faster, less data demanding methods for the less important processes. Figure 1 presents a schematic overview of the processes and methods in MIKE SHE. Detailed mathematical descriptions of the processes are available in the MIKE SHE Reference manual, which can be downloaded from the MIKE SHE web site (www.dhisoftware.com).

The flexibility in MIKE SHE's process-based framework allows each process to be solved at its own relevant spatial and temporal scale. For example, evapotranspiration varies over the day and surface flows respond quickly to rainfall events, whereas groundwater reacts much slower. In contrast, many integrated hydrologic codes (e.g. MODFLOW HMS, Panday et al., 1998; InHM, Sudicky et al., 2002) solve all the hydrologic processes implicitly at a uniform time step, which can lead to intensive computational effort for watershed scale models.

WELL HEAD PROTECTION AREAS

Well head protection areas (WHPAs) are a common planning tool for reducing the risk of contamination to drinking water supply wells (Smith et al., 2004). WHPAs are typically delineated using a calibrated steady-state groundwater flow model and deterministic backward particle tracking. Together these are used to determine the area that contributes water to the well within a prescribed time period - typically two to ten years. The WHPA then becomes subject to land-use restrictions to minimize the risk of contamination. However, conservative WHPAs are costly and WHPAs that are not conservative enough can put drinking water users at risk.

WHPAs based on steady-state groundwater models and deterministic pathlines appear smooth and accurate. Unfortunately, such capture zones ignore or simplify processes outside of the saturated groundwater zone and neglect important dynamic and transient effects, such as distributed seasonal variations in ET and net recharge, unsaturated zone storage and delayed recharge, dynamic surface water boundary conditions, high volume recharge during storms, variable pumping rates, and demand

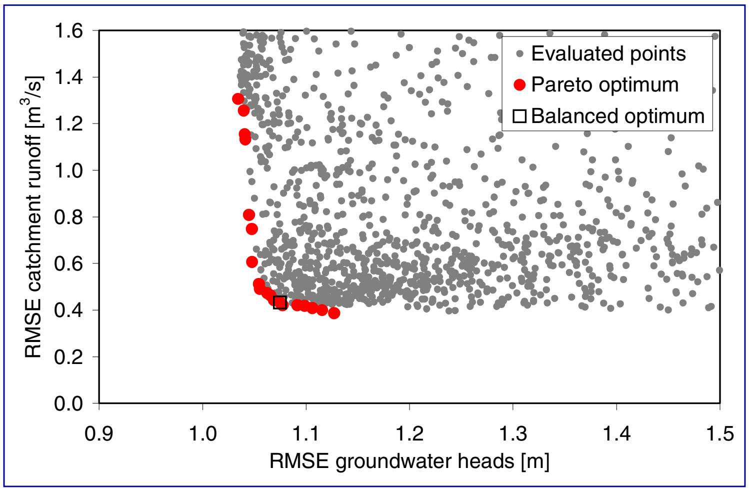

Figure 2. The balanced optimum for a two part objective function. Each dot represents the evaluation of one set of model parameters.

and land-use changes over time. Additionally, deterministic models are sensitive to uncertainty. The uncertainty arises because the mathematical process descriptions are not true reflections of the underlying physical processes. Add to this, measurement error, sub-grid scale variability of parameters, and inexact initial and boundary conditions. This inevitably leads to a range of possible models that are equally probable yet may have quite different outcomes.

Equally important for integrated hydrologic modelling is the fact that the overall time varying behaviour of the distributed model must be evaluated. In other words, the calibration must be measured against a number of possibly conflicting objectives to find an optimal calibration (assuming a unique optimum exists). In a multi-objective context, the model can be calibrated against:

- Multi-variable measurements, such as groundwater levels, river flows and water contents in the unsaturated zone,
- Multi-site measurements, such as measurement sites distributed within the catchment, and
- Multi-response modes, such as the general water balance, peak flows, and low flows.

When using multiple objectives, the solution to the calibration problem will not normally be a single unique set of parameters but will consist of the so-called Pareto set of solutions, according to various trade-offs between the different objectives (e.g. Gupta et al., 1998).

MIKE SHE includes a set of tools for automatically adjusting model parameters in response to model outcomes (Madsen, 2003). MIKE SHE's auto-calibration tool (AUTOCAL) is based on the global search, Complex Shuffled Evolution (SCE) algorithm (Duan et al., 1992). Global search methods are particularly well suited to hydrologic models because the objective function is rarely smooth with respect to the parameter values, which can cause trouble for gradient based methods.

The SCE algorithm simultaneously evolves a number of potential solutions towards the region of the global optimum of the objective function. Thus, when optimising the aggregated objective function, the SCE algorithm provides an approximation of the Pareto front (see Figure 2) near the point that corresponds to the global optimum of the objective function. By performing several independent optimisation runs with different weights, the entire Pareto front can be explored and a balanced optimum solution found.

MIKE SHE also includes a dynamic particle tracking module based on the random walk method (Uffink, 1988). The random walk method places hundreds, or even thousands, of particles in the flow field at regular time intervals. The location of every particle at each time step is a function of the current local groundwater velocity, plus a random perturbation that essentially mimics natural dispersivity. The particle tracking module keeps track of the origin, the age and the present location of all the particles. The calculated capture zone is then the locus of birth locations for the particles that were captured by the well during the simulation. Thus, a particle tracking calculation for a 10-year historic simulation will calculate the best estimate of the actual volume of water that was captured by the well during that 10 year period. The random walk method is well suited to uncertainty analysis, as the composite capture zone from series of simulations with stochastically generated data sets can be used to estimate the uncertainty of the capture zone.

THE ASSENS CASE STUDY

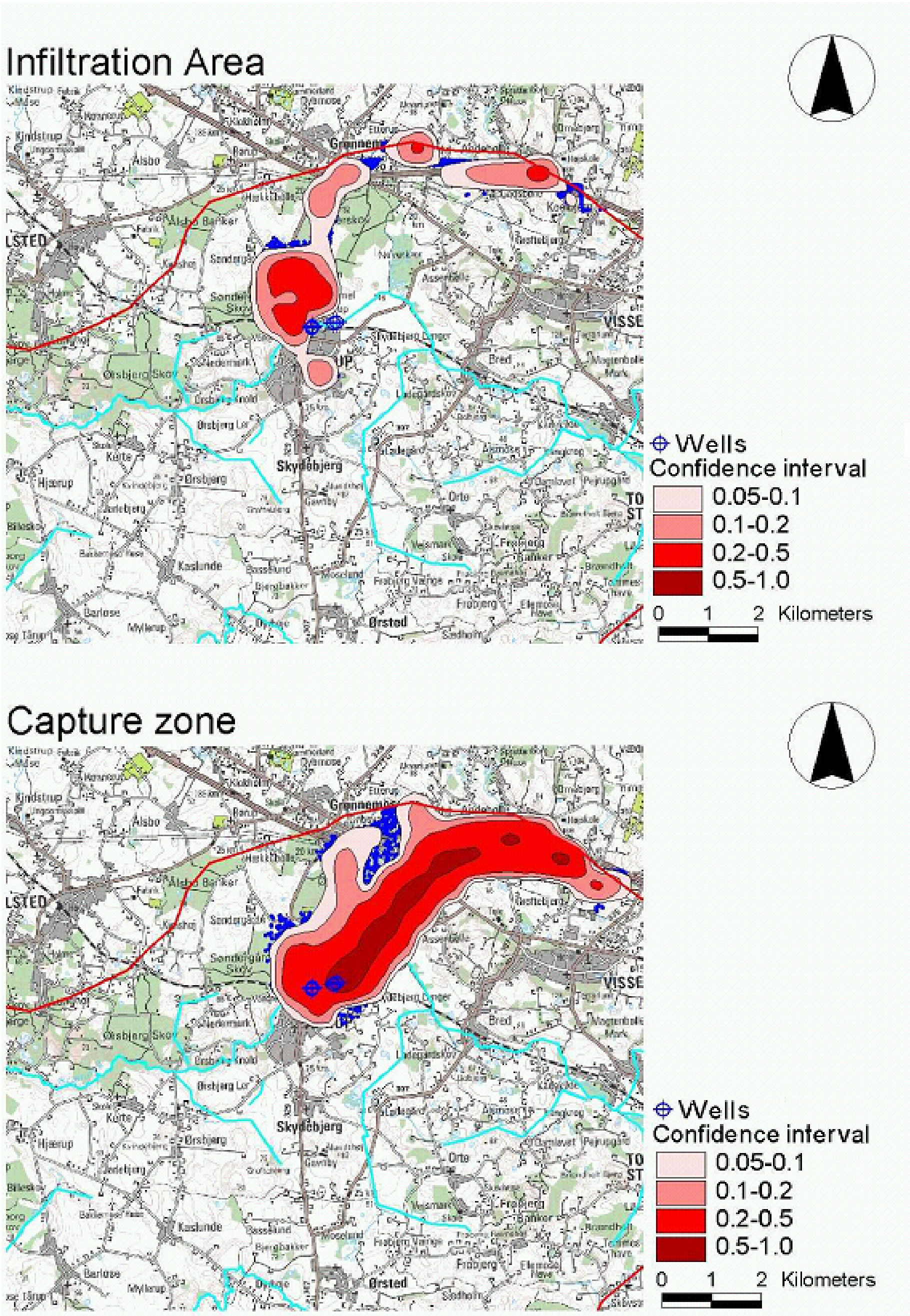

Figure 3. Composite probability map of particle capture. In the darkest areas, for example, more than 50% of all particles released were captured by the wells. The Infiltration Area represents particles starting in the top layer of the groundwater model. The Capture Zone represents the particles starting in the numerical layer containing the pumping wells.

The Assens catchment is located in the south west side of the Danish island of Fynn. The catchment is 410 km^2 with a mixture of agriculture and small urban areas. The catchment contains a network of small shallow streams, all flowing into the sea.

The Assens model was recently developed to evaluate the uncertainty associated with WHPA delineation. MIKE SHE's automatic calibration and Monte Carlo utilities were used to determine the areas that most likely contribute water to the well and, thus, optimize planning restrictions for stakeholders. The nearly 1000 simulations were distributed automatically over DHI's office network during the night to make the problem tractable.

The Assens model used the MIKE 11 kinematic routing method for flow in the streams, allowing the river flow rates to be calculated using daily time steps. The overland flow was calculated using the fully distributed finite difference method. Three-dimensional groundwater flow was calculated using a horizontal grid spacing of 500 x 500 metres. The saturated model was divided into 8 numerical layers and the hydrogeology was defined using 23 geological units. Unsaturated flow was not calculated in the Assens model. Rather it was calculated separately as net recharge using DAISY (Hansen et al. 1990) and DHI's ArcView extention DAISY GIS.

For calibration purposes, the model parameter set consisted of the horizontal and vertical conductivity for all 23 geologic units, a uniform drainage constant, and a uniform streambed leakage coefficient, for a total of 29 independent model parameters (i.e. most of the vertical conductivities were assumed to depend on horizontal conductivity). The calibration was based on a 10-year record of groundwater levels at 148 observation wells and river flow rates at five hydrograph stations. After an initial calibration, the AUTOCAL program was used to find the balanced optimum parameter set for the 16 most sensitive parameters. At the same time, the uncertainty for each of the parameter values was calculated. Based on the parameter uncertainties, a set of 85 statistically representative models were generated using Latin Hypercube Sampling. Particle tracking simulations were then made for each of the 85 models. The birth locations of all particles captured by the wells in all 85 simulations were analysed to develop a composite picture of the probability of capture (see Figure 3). That is, particles released in some areas, were always be captured. Whereas, particles released at other locations were only occasionally captured, or maybe never captured. The procedure can be summarized as follows:

1. Create the MIKE SHE model,
2. Use AUTOCAL to find the most sensitive parameters and their uncertainty
3. Generate statistically representative sets of model parameters using Latin Hypercube Sampling
4. Run MIKE SHE and the particle tracking for each model realisation
5. Aggregate the particle tracking results from all runs to determine confidence intervals for the capture zones.

The probability maps in Figure 3 also illustrate the three-dimensional nature of the capture zone. The lower map in Figure 3 is the contributing area to the well in the layer where the well screen is located. Whereas, the upper map in Figure 3 is the contributing area to the well in the top layer of the groundwater model, which represents the probable recharge area to the well.

The probability maps for the well capture zones in the Assens model are currently being evaluated by the water authorities. However, preliminary indications are that the water authority will define a primary groundwater protection area based on the recharge area defined by the 80% capture probability zones and a secondary protection zone based on the recharge area defined by 5% capture probability zone.

SUMMARY AND CONCLUSIONS

It is no longer acceptable to manage groundwater and surface water independently of one another. Advances in data collection and availability, as well as computer resources, have now made distributed, physics-based watershed modelling feasible in a wide range of applications. MIKE SHE is one of the few commercially available codes that has been widely used for integrated hydrologic modeling. MIKE SHE's process based framework allows each hydrologic process to be represented according to the problem needs at different spatial and temporal scales. Furthermore, each process can be represented at different levels of complexity. MIKE SHE has a modern, Windows-based user interface that includes advanced tools for water quality, parameter estimation, particle tracking and water budget analysis.

Well head protection areas (WHPAs) are a common planning tool for reducing the risk of contamination to drinking water supply wells. However, WHPAs delineated using a calibrated steady-state groundwater flow model and deterministic backward particle tracking do not reflect the underlying uncertainties associated with the calculations. The resulting WHPAs can be costly to implement if too conservative or put drinking water users at risk if not conservative enough.

The particle tracking and auto calibration tools in MIKE SHE can be used to calculate maps showing the probability of capture, which can be used to illustrate the uncertainty associated with capture zones. Such maps allow water authorities to define graduated WHPAs that reflect the likelihood that infiltrating contaminants will eventually impact the well. Hopefully, this will lead to greater public acceptance of the associated planning restrictions.

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