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Extended Abstracts

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5.1
Modelling as a tool of groundwater assessment

title: **Application of reactive solute transport models to groundwater risk assessment**

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INTRODUCTION

Tiered risk assessment forms a key part of the UK guidance for environmental management and pollution prevention, as part of the implementation of European and national legislation. This risk based approach is applied to management of quantity and quality of water resources, including groundwater, complies with the Water Framework Directive (EU, 2000) and is accepted by the environmental regulators (Environment Agency of England and Wales, Northern Ireland Environment Agency and Scottish Environmental Protection Agency). This tiered approach follows the source-pathway-target approach and allows for a rapid initial risk screening, through application of simplified models with inherent conservatism and comparison of the results with guideline values such as drinking water standards. If no significant risk is predicted, then compliance is assumed. Otherwise, this initial tier is followed by progression to a more sophisticated assessment, which includes a more realistic representation of attenuation processes.

For groundwater risk assessment, the first model is invariably the Environment Agency's Remedial Targets worksheet, which simulates 1-D contaminant transport including degradation and sorption (Environment Agency, 2006). This method is extremely useful because it is simple to apply and provides a rapid assessment of risk. However, it tends to overestimate contaminant concentrations and hence risks, due to the assumptions that a continuous contaminant source with a constant concentration has reached the water table and is moving directly towards the receptor.

For complex problems and a less conservative assessment of risk, more sophisticated models are required, simulating 2-D or multi-layered flow and reactive transport of dissolved contaminants, using packages such as MODFLOW (McDonald and Harbaugh, 1988) with MT3D (Zheng, 1990). Although modelling of groundwater contamination requires a fine grid and appropriate vertical resolution, in more detail than those used for most groundwater flow models, the uncertainty in the flow pattern generally has less influence on the results than the transport parameters. Thus a steady state flow model is adequate for many contamination risk assessments, based on bulk hydraulic properties, average recharge and abstraction patterns, unless the main risk drivers are preferential pathways such as fracture zones.

The MT3D code simulates reactive transport, including dispersion, first order biodegradation and equilibrium controlled linear or nonlinear sorption. When rapid predictions are required for risk assessment, published data forms the most realistic source of contaminant properties, although scaling up from laboratory or small scale field experiments remains problematic for half lives and sorption rates, and most importantly for dispersion. However, in many applications, the greatest influence on the results comes from the poorly constrained source term, with uncertain timing and mass, and on rare occasions even the location is poorly defined.

Where contamination originates from the surface above a thick unsaturated zone, significant attenuation may occur above the water table, reducing contaminant concentrations entering the saturated zone. Few of the standard modelling packages simulate unsaturated zone processes, although PHREEQC (Parkhurst and Appelo, 1999) can be used successfully for inorganic contamination when transport is dominantly through a porous matrix (Butler et al., 2003).

Two examples of local contaminant transport models are used to illustrate the approach described above, with comment on the uncertainties and outcomes for groundwater risk assessment.

EXAMPLE 1, ATTENUATION IN UNSATURATED ZONE

Prediction of fluoride concentrations and pH in a thick Triassic Sandstone aquifer were required to assess the risks and requirements for remediation, following a large spill of fluorosilicic acid, which is used to add low concentrations of fluoride to drinking water (Mott MacDonald, 2008). The Triassic Sherwood Sandstone is the UK's second most important aquifer and an important resource in northern and central England. It comprises a thick sequence dominated by poorly cemented with calcite, fine to medium grained, red sandstones, with significant primary porosity and permeability, locally enhanced by fractures.

Initial assessment, using the Remedial Targets worksheet and assuming an ongoing source of contamination, indicated possible impacts on surface and groundwater resources, beyond an agreed compliance point at a distance of 50 m from the spill. As these results were considered to be unrealistic, additional investigation and modeling were undertaken.

PHREEQC was used to approximate the movement of the fluorosilicic acid spill through the unsaturated zone, 10.5 m thick, to determine the extent of spill attenuation before reaching the water table, simulating geochemical reactions between the mineral phases and pore water solution, as well as advection. Where site specific data were not available, typical parameters were based on literature (Butler et al, 2003; Tellam and Barker, 2006). The results predicted that pH would be rapidly buffered to pH 7 and that fluoride would take 5 to 7 years to reach the water table. The predicted slow release of fluoride into the saturated zone is illustrated by Figure 1.

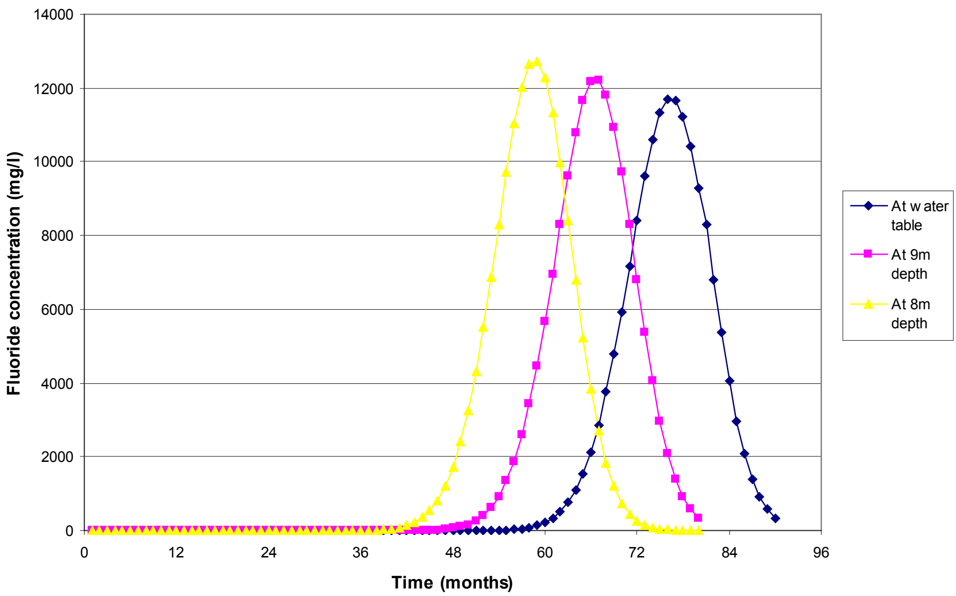

Figure 1. Simulated fluoride concentration at the water table.

The calculated concentrations were input as recharge to the MODFLOW and MT3D models, which simulated steady state flow and reactive transport using the nonlinear-Langmuir sorption isotherm, based on experimental data of average sorbed fluoride (Gresswell, 2005). The results showed that saturated zone transport of fluoride is extremely slow and that the predicted fluoride concentration exceeds the drinking water limit of 1.5 mg/l over only a small area downgradient of the site (Figure 2). Due to dispersion, a rise is concentrations at an existing monitoring well immediately upgradient of the spill is also predicted. The predictions indicate that no remediation is required to protect the aquifer beyond a distance of 150 m from the spill site.

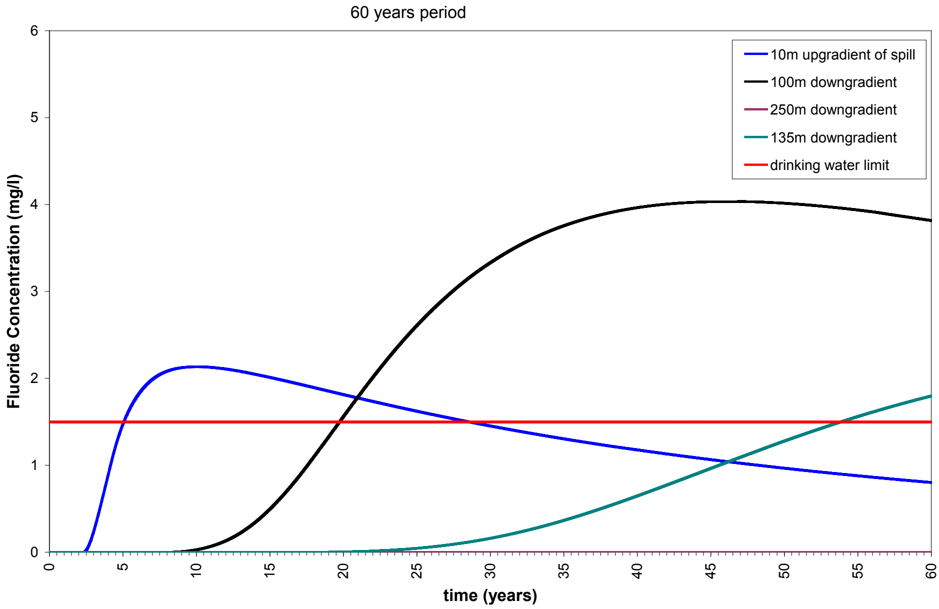

Figure 2. Simulated fluoride concentrations in the saturated aquifer.

EXAMPLE 2

The second illustration (Mott MacDonald, 2009) is an investigation into the causes of rising pesticide concentrations in an abstraction borehole, tapping the unconfined Chalk aquifer in a rural area, where both point and diffuse sources are possible but no definite sources have been identified. Thus there is uncertainty about the source's location, size and timing, as well as the thickness of the unsaturated zone. To allow for this, three alternative sources were modelled, two possible point sources (A and B) and a large area of diffuse pollution.

An initial risk assessment used the Environment Agency's Remedial Targets Methodology (Environment Agency, 2006) to simulate transport of five pesticides and identify three compounds of concern, trietazine, clopyralid and bentazone. Further modelling, using the MODFLOW and MT3D, was used to refine the risk assessment, including forecasting of the range of future concentrations. Useful data on pesticide use and properties was obtained from the European Pesticide Properties database (University of Hertfordshire, 2009). However as the location, size and concentration of the pollution sources are still uncertain and the only available data on concentrations is limited to time series at an abstraction borehole and sporadic measurements at two monitoring borehole, all models were calibrated to match modelled results to historical trends. This approach and the paucity of data result in significant model equivalence, particularly for the simple 1-D model as illustrated by Figure 3.

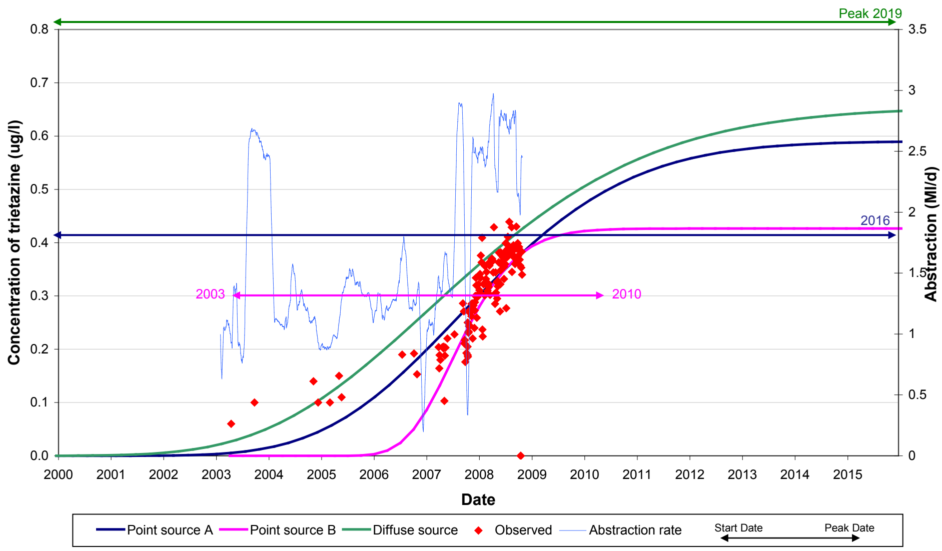

Figure 3. Simulated concentrations using simple 1-D model for 3 possible sources.

Although application of a more sophisticated approach brings a reduction in uncertainty, the inherent uncertainty in the data dominates the results. However, the results indicated that a point source is more likely than diffuse pollution, as illustrated by Figure 4, and provided a better understanding of the likely future risks even if the source is not located and remediated.

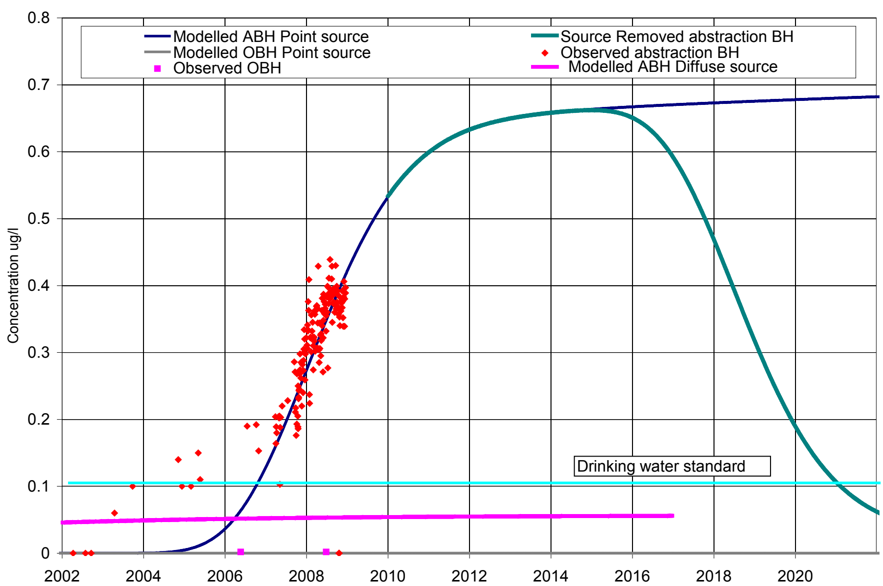

Figure 4. Simulated concentrations using 2-D model for point and diffuse sources.

CONCLUSIONS

The tiered risk assessment approach widely accepted by regulators in the UK provides a cost effective method of risk screening, but the emphasis on very simple models leads to highly conservative assumptions and overestimates of risk and impacts. In order to understand complex problems and derive a more realistic assessment, more sophisticated models are essential, including representation of reactive transport in both unsaturated and saturated zones. Results with sufficient accuracy for assessment of risks to water resources and requirement for remediation can be obtained using standard software packages, including MODFLOW, MT3D and PHREEQC, with input data based on published values to supplement site specific measurements. However, these predictions retain some uncertainty, notably when the source term is poorly understood, and would not be adequate for detailed design of remediation.

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