A system for modelling groundwater contamination in water supply areas: chloride contamination from road de-icing as an example

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Abstract A system for modelling groundwater contamination in water supply areas is presented, consisting of the flow and transport models, MACRO for the unsaturated zone and MOC for the groundwater zone, coupled to the geographical information system, IDRISI. A graphical user interface links the different parts of the system. The system was applied to a water supply area located close to a major road south of Stockholm. Chloride was used as an indicator in determining the risk for groundwater contamination from the road. The future chloride concentration in the aquifer was predicted and the effects of different pumping rates on the chemistry of the water supply well were tested. Modelling results showed that the chloride concentration in the aquifer will increase substantially due to road de-icing and that it will take decades to lower the chloride concentration down to the original background values after an end to the use of de-icing salt. The system may serve as a valuable tool in a planning context. Potential groundwater contamination scenarios can be simulated, and alternative groundwater management strategies can be evaluated.

Keywords De-icing salt; flow and transport model; geographical information systems; groundwater

Introduction

In recent years the interest for the risk of groundwater contamination from roads has increased markedly in Sweden (Bjelkås and Lindmark 1994; Bäckman 1994; Folkeson 1994; Vägverket 1995; Lindström 1996; Åhnberg and Knecht 1996; Ahnve 1997). Studies show that road constructions, traffic and road maintenance affect the groundwater quality close to roads in different ways. Effects on the groundwater quality might occur when run-off water from roads becomes polluted by car exhaust fumes, oil spills, worn particles from tyres and roads and by de-icing chemicals or by spills from accidents infiltrating into the groundwater. The problems that mostly affect the groundwater resources close to roads are the last two; viz. the de-icing salt and accidents that release petroleum products and/or other toxic liquids (Bjelkås and Lindmark 1994; Folkeson 1994; Lindström 1996; Eliasson 2001). The application of de-icing salt may also cause secondary effects for the roadside environment, such as increased mobility of metals (Amrhein *et al.* 1994; Norrström and Jacks 1998), as well as a reduced acid neutralising capacity in surface water by ion exchange (Löfgren 2000; White *et al.* 2000).

Chemical de-icing with sodium chloride (NaCl) on roads has been used in Sweden since the mid-1960 s (Bäckman 1994). Studies carried out in a number of test areas show that highway de-icing using NaCl may cause raised salt levels in the vegetation, soil and groundwater along roads. Under certain conditions this can also lead to damage of the vegetation (Blomqvist and Johansson 1999; Viskari and Kärelampi 2000) and to pollution of surface water and groundwater (Johansson Thunqvist 2003). Effects of de-icing salt have

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been shown in municipal water supply wells (e.g. Maxe *et al.* 1994; Planting 1997; Knutsson *et al.* 1998; Rosén *et al.* 1998; Müllern 2000) as well as in private wells (e.g. Fabricius and Olofsson 1996; Olofsson and Sandström 1998; Gustafsson and Nystén 2000; Gontier 2001). It has been found that the hydrogeological conditions are a significant factor when considering the influence from applying de-icing salt (Soveri 1992; Tuominen 1994; Bäckman 1994).

In the present study a system for modelling the risk for groundwater contamination in important water supply areas is presented, consisting of a one-dimensional flow and transport model for the unsaturated zone MACRO (Jarvis 1994); a two-dimensional model for the groundwater zone MOC (Konikow and Bredehoeft 1978; Goode and Konikow 1989) and a geographical information system, IDRISI (Eastman 1992, 2001). The components work separately but programming was done in the groundwater model code to get an easier exchange of input and output files with the GIS. Furthermore, a graphical user interface was developed to facilitate the joint use of the three components.

The use of separate models for the unsaturated and saturated zones implies simplicity and flexibility to the system compared with a fully integrated 3D unsaturated–saturated modelling system. In areas with sand and gravel and with a deep groundwater table with relatively small variations, as in typical Swedish water supply areas, a one-way downward water transport from the unsaturated to the saturated zone is dominating and the use of separate models for the two zones can be justified. The choice of a 2D or 3D model of the saturated zone has to be based on the local hydrogeological conditions. If no data on clear vertical stratigraphy or vertical differences in hydraulic parameters exist and the horizontal extent of the study area is much larger than the thickness of the saturated zone, the use of a 2D model is motivated.

In order to determine if groundwater quality is threatened by road de-icing, it is important to reveal trends for the salt concentrations in the aquifers and to predict future salt concentrations. Furthermore, quantification of the effect of remedial measures is needed. The main objective of the present study was to assess the vulnerability of an important groundwater supply area in Haninge municipality, south of Stockholm, in terms of travel times and chloride concentrations using predictive models. The paper also describes the primary components and the features of the groundwater management system that was used for the predictions. The aquifer had earlier been subjected to detailed investigations by VIAK AB (1990) and by SGU (Müllern 1993).

Materials and methods

The system used was built up from existing software and the main effort was placed on linking the software. Hence the models and included parameters are not discussed in detail.

The flow and solute transport in the unsaturated zone was simulated using a one-dimensional vertical model for macroporous soils, MACRO (Jarvis 1994). The model can simulate canopy interception and washoff and plant uptake, convective-dispersive transport sorbing and degrading solutes. Moreover, MACRO accounts for preferential flow occurring in structured soils. A number of options in the model allow the user flexibility in matching the simulation to the particular conditions that are of interest. The most important options relate to precipitation input (hourly or daily rainfall data), the type of solute and the type of vegetation. Owing to the one-dimensional nature of the model, multiple realisations are needed to account for the horizontal variations in the unsaturated zone.

Output data (daily values of fluxes and solute concentrations) from the MACRO model were used as input into the two-dimensional horizontal model, MOC (Konikow and Bredehoeft 1978; Goode and Konikow 1989), for modelling of groundwater flow and transport. The model incorporates a first-order, irreversible rate reaction, linear and non-linear equilibrium-controlled sorption and equilibrium-controlled ion exchange. Numerical procedures incorporate these processes in the general solution scheme that uses methods-of-characteristics with particle tracking for advection and finite-difference methods for dispersion. A particle tracking routine, allowing both forward and backward tracking, was developed for the model in the present project.

The groundwater model was linked to the geographical information system (GIS), IDRISI (Eastman 1992, 1995), which is used for the preparation of input data and presentation of output data in the form of maps. IDRISI is able to further analyse the results by, for example, using the overlay technique. The raster-based IDRISI is flexible due to its modular structure and the possibility for batch and meta programming, as well as for construction of new modules. In the present study, the flow and transport models were kept separate from IDRISI, resulting in a less interactive, but more flexible system.

A graphical user interface was developed to link the modules and facilitate the use of the system. The user is guided through the application and the modules are connected in a way that gives the user an impression of using one single software.

Description of the Jordbro study area

The study area is shown in Figure 1. The Jordbro aquifer is situated in Haninge municipality, south of Stockholm. The main groundwater supply for the Haninge municipality lies in the Stockholm esker that runs in a south–north direction through Hanveden and Jordbro. Today the water supply well in Jordbro is not in use, but there have been plans to pump groundwater from the well to the Hanveden water supply site downstream in the same esker in order to safeguard the water quality and quantity of groundwater in Hanveden. It has been planned that 7.5 L/s of groundwater from the Jordbro well will support artificial recharge in the water supply well in Hanveden.

The Jordbro formation, which consists of gravel and sand, is highly permeable. The thickness of the esker deposits, that underlie the entire study area, varies between 10–30 m across most of the area. The thickness of the unsaturated zone varies between 2–10 m. Precipitation (550 mm/yr) is considered to be the only source for groundwater recharge. The stream along the eastern boundary is characterised as effluent. Annual average groundwater recharge in the central part of the area is estimated at 140 mm. The relatively low estimated

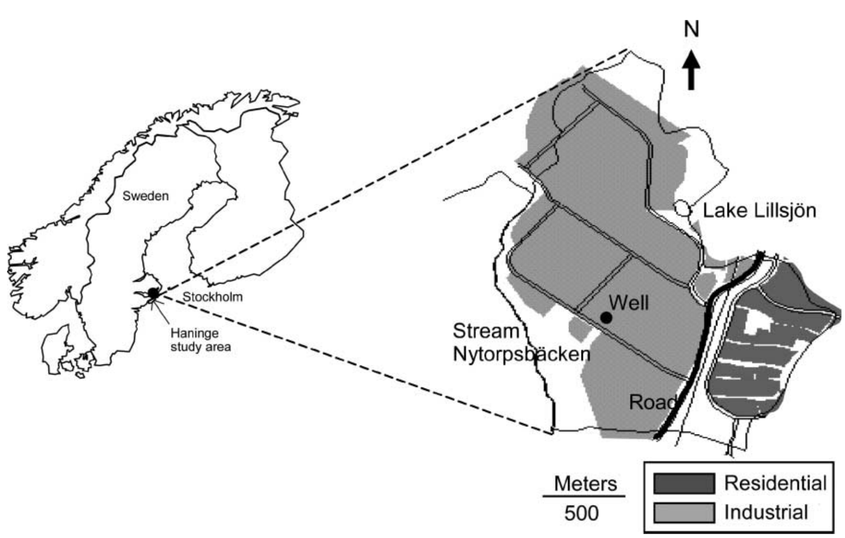

Figure 1 The Jordbro study area. Dark shaded areas show residential areas and the light shaded area shows the Jordbro industrial area

recharge is motivated by the industrialisation (VIAK AB 1990). In surrounding areas the recharge is estimated at 315 mm/yr except for the residential areas where the recharge is estimated at 230 mm/yr. The groundwater recharge area is approximately 2–3 km^2.

The road Nynäsvägen transverses the area over a distance of 1.5 km along the esker formation. Under natural conditions the groundwater flows to the northeast from the road and not towards the water supply well.

Storm water from the industrial area is directed to the stream Nytorpsbäcken and to Lake Lillsjön, which lies in the northern part of the area. Under undisturbed conditions the groundwater table in the aquifer is relatively flat with a small gradient in a northerly direction. The discharge from Lake Lillsjön is 9 L/s with a large proportion being groundwater from the Jordbro aquifer.

A pumping test was performed in the planned water supply well over a period of two years, from July 1987 to July 1989. The pumping rate from the well was 13 L/s during the entire pumping period. On the basis of the pumping test, the transmissivity was estimated to 1×10^{-2} m^2/s (VIAK AB 1990).

During the pumping test, water quality was analysed on several occasions. Chloride concentrations showed a clear increasing trend but stabilised at 90 mg/L after two years' abstraction. Except for the two years' long pumping period, no water has been abstracted from the planned water supply well.

Conceptualisation and model setting

The general simulation procedure is illustrated in Figure 2. In the present study the transport of chloride from the road through the unsaturated zone and the further spreading in the groundwater zone was simulated and future chloride concentrations predicted.

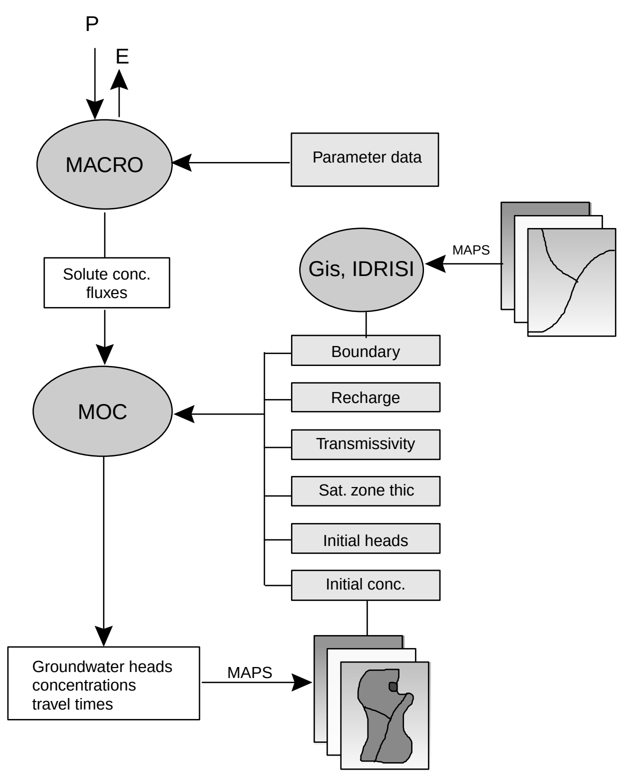

Figure 2 Graphical illustration of the system used in the study

It was assumed that the unsaturated zone conditions were constant along the whole stretch of the road. Therefore, only one simulation using the MACRO model was needed for the road area. The initial chloride concentration (not affected by de-icing salt) of 25 mg/L in the groundwater was based on earlier measurements in the observation wells. Furthermore, the initial concentration in the unsaturated zone was assumed to be the same as in the underlying strata. The thickness of the unsaturated zone along the road was assessed to be 5 m. The width of the road was set at 10 m, and the width of each of the roadside ditches was set to 1 m. Road salt (10 kg/m/yr) was applied on the road during the period November to March. Salt application was assumed to take place during days when the daily temperature was around 0°C. An assumption was made that precipitation falling on the road would flow equally into the two roadside ditches and be infiltrated. The amount of de-icing salt used varies from season to season. The salt application rate assumed in this study is normal for the actual road maintenance category. Snowfall/snowmelt was not included in the simulations. In this case, it was assumed that road de-icing salt would melt the snow in the roadside ditches, allowing infiltration into the soil during winter.

As input data to the MACRO model, daily values of the precipitation and evapotranspiration from SMHI (Swedish Meteorological and Hydrological Institute) were used. Field parameters were taken from a database version of MACRO, MACRO-DB (Jarvis *et al.* 1997). The MACRO simulation gave daily values of the water flux and the chloride concentration entering the groundwater zone. The resulting time series were used as input into the MOC model, together with the hydrogeological data prepared by IDRISI. The models were linked through fluxes, which provide a match in the mass balances between the models. However, this leads to the potentials at the coupling depth to be mismatched. It was assumed that there were no upward fluxes at the coupling depth of 5 m below the surface. This was considered reasonable due to the relatively deep location of the groundwater table. In the present application, the groundwater model worked without any back-coupling to the MACRO model.

The MOC code was modified for easier exchange of data with IDRISI. Using raster routines in IDRISI, a finite-difference grid was constructed. One pixel (20 × 20 m) in IDRISI corresponded to one cell in MOC. Input data files, stored as maps in IDRISI, consisted of boundary conditions, initial head, initial concentration, groundwater recharge, transmissivities, thickness of the saturated zone and node identifications.

Eastern and western boundaries for the simulated area were defined by the boundary of the esker formation. The surrounding deposits mainly consist of till and clay. The western boundary runs along the stream Nytorpsbäcken in a north–south direction, while the northern and southern boundaries follow the topography of high bedrock areas and were defined as no flow boundaries. It was more difficult to define the eastern boundary, which consists of wetland areas. Here the groundwater was assumed to have constant head.

For simulations of salt transport from the road Nynäsvägen, the transmissivity was calibrated to known groundwater heads in six observation wells. The calibration was performed manually by trial-and-error adjustment of T values. Results from each model execution were compared to the measured heads in observation wells to obtain the best fit between measured and simulated heads. For the finally selected T distributions the total root mean squared (RMS) error in measured and simulated heads was 0.11 m. Calibrated transmissivities varied between 1×10^{-2} to 1×10^{-4} m^2/s, the higher values for the central part of the esker with the coarsest material. Boundaries and transmissivities are shown in Figure 3. The effective porosity in the aquifer was set to 30%.

Empirical values were used for dispersion. The longitudinal and transverse dispersivity was estimated as 10% (60 m) and 1% (6 m) of the flow-path length, respectively.

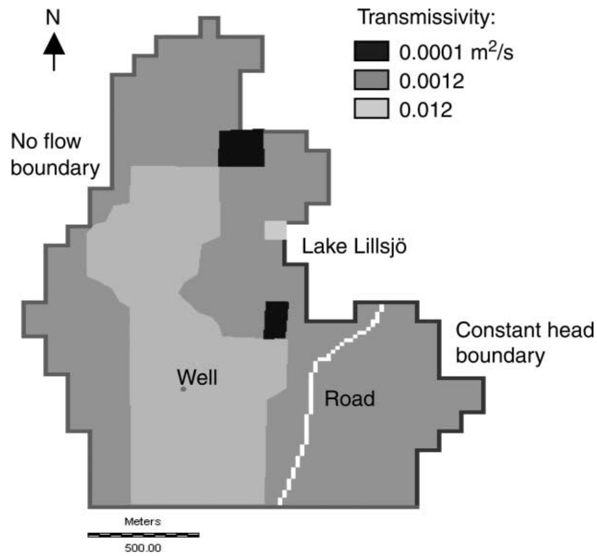

Figure 3 Transmissivities and boundary conditions for the study area in the Jordbro aquifer

To test the model chloride data from the pumping test was used. The pumping rate in the test simulation was set to 13 L/s as in the pumping test. The maximum simulated chloride concentration in the well was approximately 60 mg/L – a level reached after 3 years of abstraction. During the two year long pumping test, chloride concentration in the well varied between 60 mg/L and 100 mg/L, the lower concentrations occurring during the summer period. The results from the modelling were hence somewhat lower than the measured concentrations and the maximum concentration was reached later in the modelling exercise.

In the final scenario chosen for the study, based on the plans of the municipality, the abstraction rate was set to 7.5 L/s, which corresponds to natural mean groundwater recharge in the area.

Results

Precipitation, water fluxes and chloride concentrations from MACRO simulation for the unsaturated zone for a four-year period are presented in Figures 4, 5 and 6. The fluxes shown are only those in the roadside ditches.

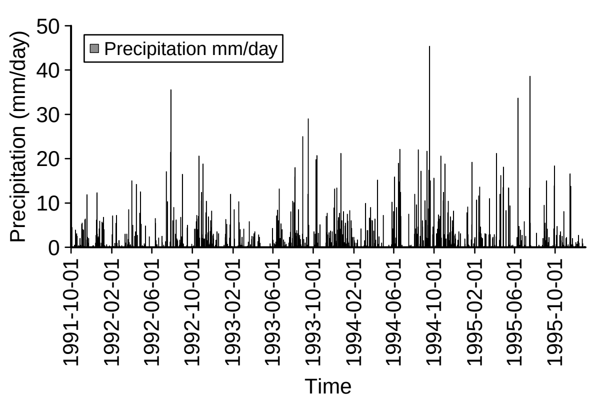

Figure 4 Precipitation during 1991–1995 in the study area

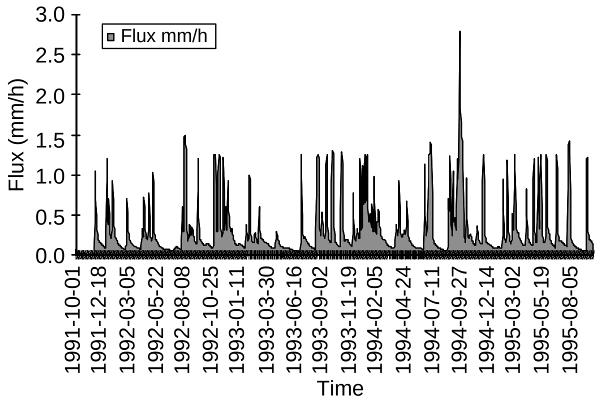

Figure 5 Fluxes of infiltration water into the saturated zone in the roadside ditches simulated by MACRO during 1991–1995

The accumulated yearly water flux and the maximum concentration under the road were 1314 mm/yr and 3600 mg/L, respectively. The yearly flux is higher than the precipitation as the flux in the roadside ditches was assumed to consist of precipitation falling on the road and gathering the precipitation from the road area. Variations in the chloride concentration simulated by the MOC model for a 10-year period in the aquifer at a distance of 100 m and 300 m from the road are shown in Figure 7.

Figure 8 shows a map of the groundwater level in the aquifer at a pumping rate of 7.5 L/s. Particle tracking from the road is also shown. Figure 9 shows chloride concentrations in the aquifer after ten years' application of de-icing salt at a rate of a 10 kg/m/yr, the initial chloride concentration being 25 mg/L and the abstraction from the water supply well being 7.5 L/s. After ten years, according to the model simulation, the chloride concentrations in the aquifer 100 m and 300 m from the road were about 110 mg/L and 58 mg/L, respectively, while the concentration in the water supply well was about 30 mg/L. The water supply well is located approximately 600 m from the road and will be affected by the de-icing salt after about 8 years. In the second scenario, illustrated by Figure 10, road de-icing has been carried out for a period of ten years and then stopped for a ten-year period. Notably, in the scenario in which salt application was stopped after 10 years, there was a maximum chloride concentration of about 60 mg/L in the water supply well. This maximum concentration was reached nearly 5 years after halting the application of de-icing salt.

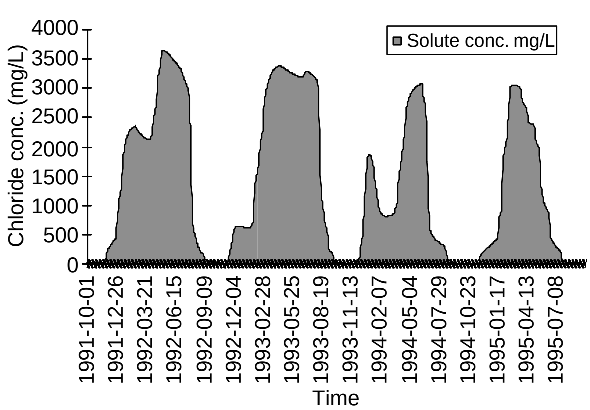

Figure 6 Chloride concentrations in the infiltration water into the saturated zone in the roadside ditches simulated by MACRO during 1991–1995

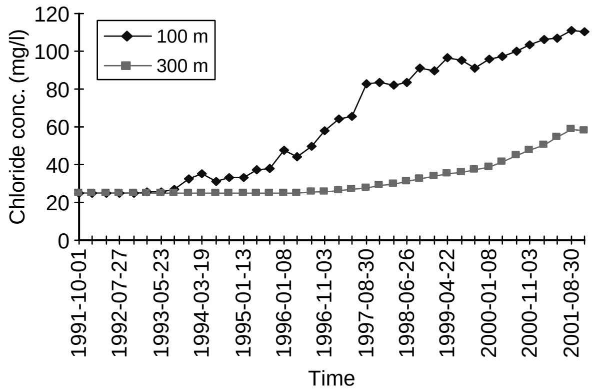

Figure 7 Variation of modelled chloride concentration in the aquifer at 100 m and 300 m from the road

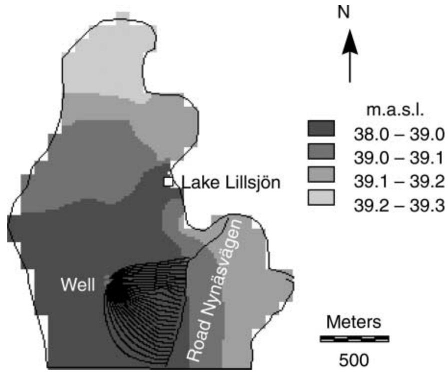

Figure 8 Groundwater levels and particle tracking lines resulting from a pumping rate of 7.5 L/s in the water supply well

Discussion and conclusions

The results of the study demonstrate the potential usefulness of the presented system as a tool for the evaluation of the impact of road de-icing on groundwater quality, and for assessing changes in groundwater quality due to different remedial measures, such as reducing salt application. Because of the conservative nature of chloride, it is a good tracer and hence it can show potential contamination in the subsurface also for other water-soluble contaminants, whose travel times and concentrations are affected by sorption and decay.

The MACRO model applied in the present study may be regarded as unnecessarily advanced for the study of chloride transport. Often approximate analytical solutions, for

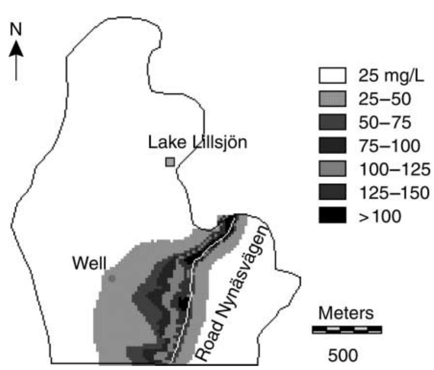

Figure 9 Chloride concentrations in the aquifer after 10 years application of de-icing salt

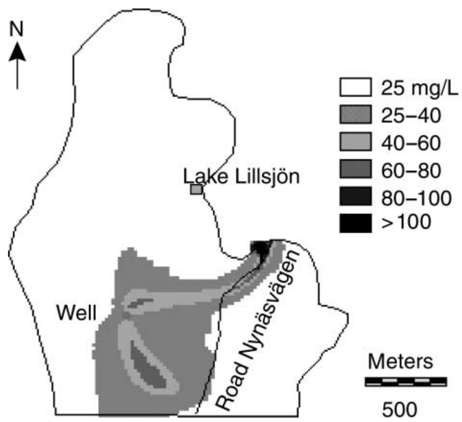

Figure 10 Chloride concentrations when de-icing salt has been applied for 10 years and then stopped for 10 years

example by Green and Ampt (1911), are used for the prediction of convective transport in unsaturated soils. However, if reactive contaminants are to be studied models including at least sorption and decay processes are needed.

For spills of petroleum products, a relevant scenario in a road context, MACRO should be substituted in the system by a NAPL model, while MOC could still be used to simulate the transport of dissolved parts in the saturated zone.

In the case study, the maximum chloride concentrations after 10 years of salt application was 110 mg/L and 58 mg/L at 100 and 300 m distance, respectively, from the road Nynäsvägen. It took approximately 8 years until the water supply well, located 600 m from the road, was affected. Despite halting the application of salt after 10 years, the chloride concentration in the water supply continued to rise for a period of 5 years and reached a maximum concentration of 60 mg/L. A further 10 years after stopping the application of salt, the chloride concentration was still well above the background concentration. The technical drinking water limit of 100 mg/L was exceeded at a distance of 100 m from the road but not in the well water. In the vicinity of the road, chloride concentrations were even higher. According to the model simulations, the chloride concentration in the aquifer varies annually and seasonally both in the unsaturated and in the groundwater zone. The seasonal variation in the groundwater zone occurs mainly close to the road, but can still be identified 100–200 m away from the road. When the salt plume advances further away from the road, dispersion implies declining seasonal variation.

Comparison of the modelled results with the measured concentration in the well during the pumping test showed that a somewhat slower response and lower concentrations were obtained with the model predictions. The cause of this may be the relatively high effective porosity value and relatively high longitudinal dispersion used in the model. Lower effective porosity results in faster transport of chloride to the well and lower dispersion values give higher concentrations. In order to define the dispersivity values and effective porosity values correctly, collection of more field data is needed.

The focus of the present study was mainly on the linkage of several computer programs to a system for modelling groundwater contamination and, therefore, no thorough sensitivity analysis of the results of the case study was carried out. However, such a study is strongly recommended before the results are used for planning and management purposes.

A merit of using the present modelling approach, compared to the index methods often used in groundwater vulnerability assessment (Vrba and Zaporozec 1994; Lindström and Scharp 1995), is that the results are quantitative, for example in terms of concentrations, critical load and/or travel times. However, the modelling approach is data-demanding. When input data are scarce, the results obtained will suffer from uncertainty. Therefore, procedures for carrying out uncertainty assessment should be included. Ideally, all data used for the modelling should be site-specific. Generic data should only be used if collection of site-specific data is not possible.

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