

Application of flow and transport models to the polluted Honkala aquifer, Säkylä, Finland

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High concentrations of tetrachloroethylene were discovered in groundwater samples taken from the Honkala aquifer in the municipality of Säkylä in southwestern Finland. The contamination was traced to a dry-cleaning laundry located close to a tributary esker which is connected to the Säkylänharju esker in the northeastern part of the area. The Weichselian and Holocene sediments of the area include till, sand and gravel and also glacial and postglacial clay deposits. The groundwater flows west towards Pyhäjärvi (a lake in the municipality of Säkylä). A study was launched to test the applicability of numerical groundwater models in developing an overview of groundwater flow and contaminant transport in the area and prediction of the timing of natural attenuation. Modelling was conducted with the MODFLOW, MODFLOWP and MT3D codes, the resulting simulations indicating a natural attenuation time of more than 30 years would be required for the aquifer. Active aquifer restoration would require pumping and treatment of the polluted groundwater.

Introduction

Groundwater is an important natural resource, and almost 60% of all the drinking water supplied by waterworks in Finland is either natural or artificially recharged groundwater (Finnish Environment Institute 1999, 2001). Groundwater resources are protected under environmental law in Finland, and their pollution is strictly forbidden.

There have been many reported cases of groundwater pollution in Finland (see Nystén 1988, Salonen *et al.* 2001), and numerical models of groundwater flow and contaminant transport have been applied to such cases, e.g. instances of pollution by road salting (De Coster *et al.*

1993, Nystén *et al.* 1995), chloride from a landfill (Ahlberg and Soveri 1988, 1991) and chlorophenols from a sawmill (Nystén 1994). As shown in these previous studies, typical Finnish aquifers are vulnerable to such accidents by nature, as they are mostly shallow and unconfined, with low biochemical activity. Groundwater flow and contaminant transport models have proven useful for predicting the effects of pollutants in groundwater.

The restoration of an aquifer is often difficult, because the subsurface environment cannot be described and characterized precisely enough. In an environment with a rather thin, heterogeneous glaciofluvial cover, the topography

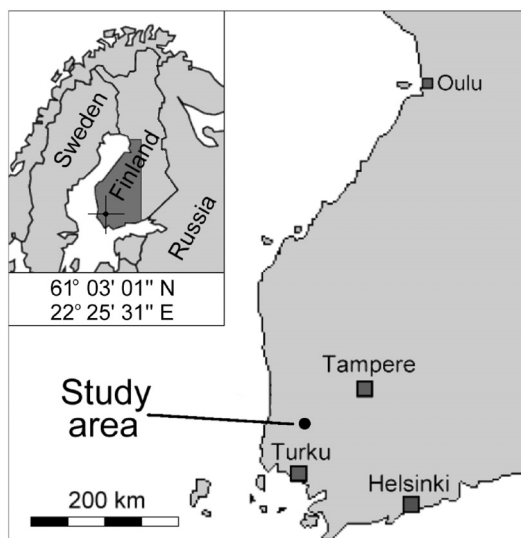


Fig. 1. Location of the study area.

and structures of the almost impermeable crystalline bedrock are important issues influencing groundwater flow. Moreover, heterogeneity in the Quaternary sediments can result in significant variability in the hydraulic properties of aquifers at different scales.

The area of concern is located in the municipality of Säkylä in southwestern Finland (Fig. 1). In August 1998, a large variety of chemical analyses were made on groundwater samples taken from the old municipal waterworks, located in the Honkala groundwater area (Lounais-Suomen ympäristökeskus, unpubl.). Large concentrations of tetrachloroethylene (PCE) and minor concentrations of trichloroethylene (TCE) were found in these samples, the source of the PCE being identified as a dry-cleaning laundry three kilometres away (Artimo 2001), which had been using the chemical for more than 30 years.

This study was launched in order to obtain sufficient information on the aquifer to support its restoration and to protect the local inhabitants from the effects of the pollutants. A numerical groundwater flow model and a contaminant transport model were employed to interpret the flow system of the Honkala esker aquifer and to predict the time needed for natural attenuation to reduce contaminant concentrations below acceptable drinking water limits.

The Honkala esker area

The main aquifer in the area is composed of esker deposits (Fig. 2), which formed during the Late Weichselian deglaciation of the Scandinavian Ice Sheet. It is mostly unconfined, and only partly confined in the zones where the esker is covered by marine clays and silts.

The bedrock topography and the thickness of the glacial drift in the vicinity of the study area vary markedly, as discussed by Lindroos *et al.* (1983). The Honkala area is a part of a larger area for which a groundwater flow model has been constructed by the Southwest Finland Regional Environment Centre. This regional-scale model was not accurate enough to meet the demands of the present investigation, however (Mäkinen and Seppälä 2001), and it had omitted parts of the Honkala area because of a lack of data. New data obtained from the present work defined the previous conceptual model more closely, and resulted in a new refined representation of the Honkala aquifer.

Research material

The modelling effort called for a large body of field data. Chemical analyses for PCE and its degradation products (under reducing conditions), including TCE, dichloroethylene and vinylchloride were carried out on 107 groundwater samples (Fig. 3). The first 28 samples were analyzed with a gas chromatograph–mass spectrometer (P&T/GC-MS) at the Laboratory of Chemical Technology at the Technical Research Centre of Finland. The method is accredited (KET1201195). The other 79 samples were analyzed in the laboratories of the Institute of Occupational Health in Turku, with a gas chromatograph equipped with an electron capturing device (GC-ECD). In order to ensure equivalence between the results, some parallel samples were sent to both laboratories before the last series of 79 samples were analyzed only in the laboratories of the Institute of Occupational Health.

Hydraulic heads in 65 wells were measured (Fig. 3), and four multi-level monitoring and sampling wells were constructed to complete the

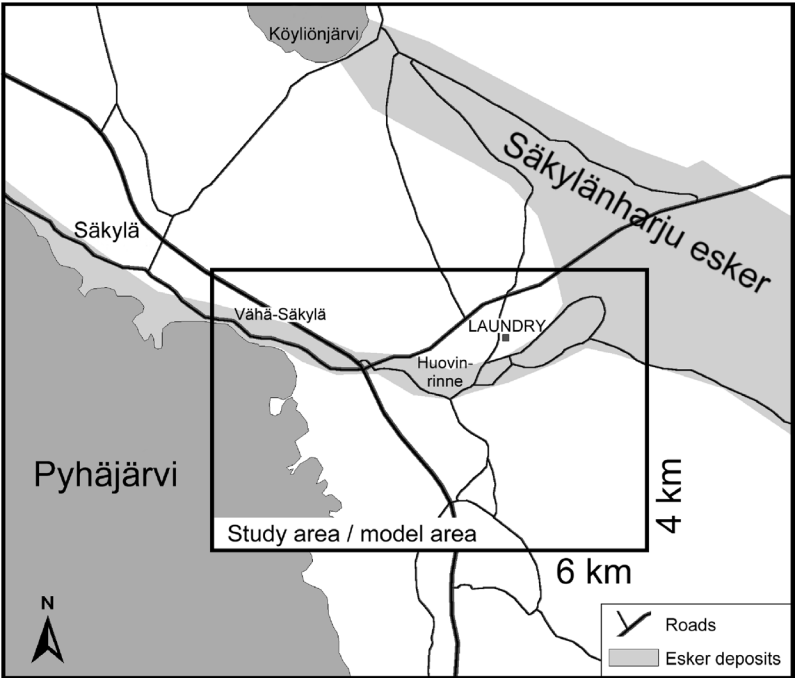


Fig. 2. Outline of the area studied and modelled and of the extent of the Weichselian esker deposits hosting the aquifer.

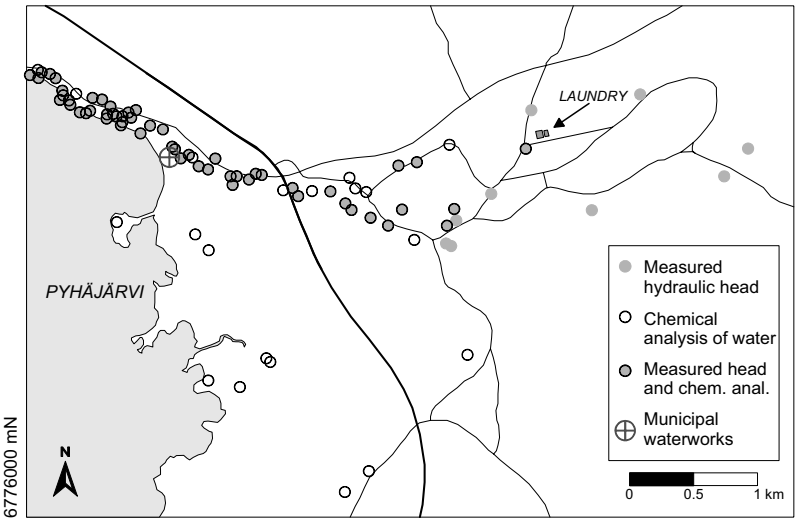


Fig. 3. Locations of the municipal waterworks, wells, and monitoring wells in which hydraulic heads and/or concentrations of PCE and its degradation products were measured.

observation network in the contaminated area (Artimo 2001).

The elevation of the bedrock was interpreted from gravimetric measurements (A. Mattsson, unpubl.) and drilling data, including 17 gravimetric profiles with a total length of 12 680 metres (Fig. 4). The measurements were cali-

brated by means of rotary drillings performed at the ends of the profiles. Bedrock properties — including rock type, level of weathering, and fragmentation — were examined from hand-specimens taken at drilling locations K1 to K8 and HP1 to HP4 (Fig. 4). The hydraulic conductivity of the bedrock in the sandstone area was

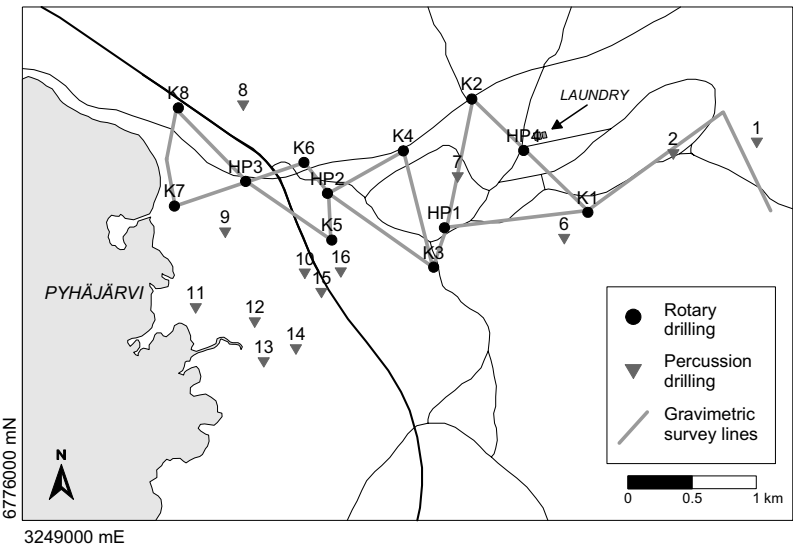


Fig. 4. Locations of new drilling sites and extent of gravimetric measurements.

measured from one sample (HP3) with flexible wall permeameter. The other bedrock samples in the sandstone area were clearly disturbed. In addition, 12 percussion drillings were made to map the extent of sandy units around the esker (Fig. 4). This drilling equipment did not provide a possibility to collect samples of the unconsolidated deposits, and the interpretation of the soil properties was based on the observed penetration rate of the drill stems.

Previous research data, including water level monitoring data from 9 locations, were also used. These data covered several years of monthly monitoring. The annual variation of the flow system in the Honkala esker aquifer is quite limited, the average variation in measured hydraulic heads being about 0.5 metres within a year. The maximum recorded water level variation in one monitoring point has been 1.92 metres. Largest variations occur in the areas of fine-grained sediments. Nevertheless, the groundwater flow patterns remain quite consistent year-round.

The aquifer parameter values used in the flow and transport model were mostly obtained from the literature (e.g. Freeze and Cherry 1979, Kling *et al.* 1993, Zheng and Bennett 1995), and from the field observations. For instance, the observed soil type and grain-size distribution in the study area were used to control the parameter input values.

In the areas where the layer 2 of the model represents weathered and fractured bedrock, given hydraulic conductivity values vary from 5×10^{-5} to 1×10^{-1} (m d⁻¹). These values were based on the observations of hand-specimens and on the magnitude of the measured conductivity of the sandstone sample.

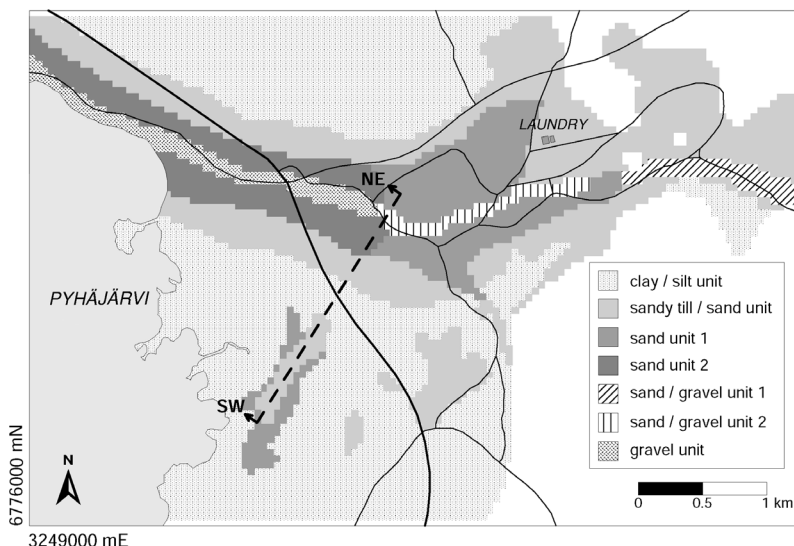
Layer 2 has also higher hydraulic conductivity values in the area where the layer was used to simulate confined groundwater flow in unconsolidated deposits. The aquifer parameter values are presented in Table 1.

The timing of the pollution was based on the fact that the underground storage tanks of the

Table 1. Range of aquifer parameter values. Hydraulic conductivity values represent initial values for inverse modelling with MODFLOW.

Hydraulic conductivity (m d ⁻¹)	Effective porosity	Longitudinal dispersivity (m)	Transverse dispersivity (m)	Aquifer thickness (m)
5×10^{-5} –100	0.05–0.25	40–50	4–5	0–55

Fig. 5. Zones (hydrogeological units) used in calibration in order to differentiate the spatial distribution of hydraulic conductivity in the upper layer of the model. The zones represent units in which the ratios of given K-values within that unit remain the same. Initial values of hydraulic conductivity in the upper model layer vary from 0.1 to 100 m d⁻¹.



dry-cleaning laundry had been replaced in the late 1970s because of observed tetrachloroethylene leaks. PCE consumption rates reached their peak in 1976–1977, after which annual consumption has been 30%–75% lower. These data led to the conclusion that the leak had occurred within the years 1976 and 1977. However, the precise amount of the leaked chemical can not be concluded from the recorded consumption rates of PCE, because unknown amount of the purchased chemical was stored for later use. Nevertheless, the estimated amount of leaked PCE can still be measured in hundreds or thousands of kilogrammes according to the observations of the laundry's former employees.

Methods

The first aim was to construct a numerical groundwater flow model based on the MODFLOW code (McDonald and Harbaugh 1988) in order to interpret the flow system of the aquifer, and to calibrate it with the MODFLOWP code (Hill 1992), which uses the inverse modelling technique. The second aim was to build a solute transport model on the basis of the calibrated flow model in order to evaluate total concentrations of PCE over the whole modelled area and the possibilities for remediation processes. MT3D code was chosen for solute transport modelling.

The hydraulic head monitoring data was scarce and the measurements in all the 69 locations were made only once. However, some of these monitoring sites were later included into monthly observation program along with the 9 previous monitoring locations. Incomplete observation material over a longer period of time resulted in a steady state flow simulation. Steady state simulation was considered to represent the aquifer flow system precisely enough based on the earlier observations of seasonal variation in hydraulic head.

Spatially distributed quantities such as hydraulic conductivity and areal recharge can be defined using zones of constant value, interpolation methods, and some stochastic methods (Hill *et al.* 1998). In the present case an interpretation of the depositional characteristics of the modelled area (J. Mäkinen, pers. comm.) was introduced into the calibration scheme by the zonation method of automatic calibration in order to identify the spatial variability of hydraulic conductivity in the aquifer (Koltermann and Gorelick 1996). In this procedure, the aquifer was divided into zones representing depositionally consistent areas; i.e. the hydrogeological units of the aquifer were introduced into the calibration scheme (Fig. 5). This reduces the number of parameter values, and the smaller-scale hydraulic property variations can be represented within zones (Anderson 1989). MOD-

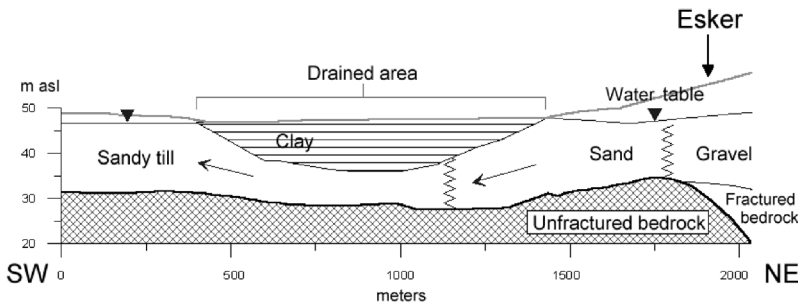


Fig. 6. Schematic profile of the confined part of the aquifer. The location of the cross-section is presented in Fig. 5.

FLOWP was used to calculate the factor for hydraulic conductivities within each zone in order to match the model with the physical system of the study area.

Impermeable bedrock formed the lower boundary of the modelled system. Pyhäjärvi on the western side of the modelled area penetrates the aquifer and was treated as a specified head boundary. The aquifer consists of tributary esker connected to the Säkylänharju esker in the north-eastern part of the area (Fig. 2). Specified head boundaries in this area were determined from field information. Northern and southern boundaries of the model are located in the clay area, where the hydraulic head is mainly controlled by the drainage systems.

The depositional characteristics of the area clearly indicated the influence of intersecting bedrock fractures on the deposition of esker material in the middle part of the modelled area and on the groundwater flow conditions, as also seen by Salmi (1978) in the Virttaankangas–Mellilä esker. Other changes in bedrock topography have also been reported to influence the deposition of esker material in the area (Lindroos *et al.* 1983).

The solute transport model (MT3D) was based on the calibrated flow model, and the transport modelling was made with trial-and-error method on account of the scarcity of initial data. The amount of tetrachloroethylene introduced to the solute transport model was based on the estimations of leaked chemical, calibration results, and on comparisons with the measured PCE values. Longitudinal and transverse dispersivity values (α_L and α_T) were also estimated during the calibration as well as the effect of sorption. Radioactive decay and biodegradation were not simulated in the model.

Results

The conceptual model was mainly constructed on the basis of the depositional characteristics of the area combined with drill-log data and hydraulic head observations. These data were adequate for the characterization of the main hydrogeological units (Fig. 5). The observed distribution of PCE in the groundwater also provided information on groundwater flow connections. Schematic profile of the confined part of the aquifer is presented in Fig. 6.

Soil porosity in the area is estimated to vary from about 0.1 to 0.65, these minimum and maximum values being those representing the porosities of till units and clays respectively. Porosity in the esker area itself varies from 0.25 to 0.3. Alternatively, effective porosity may be said to vary from 0.08 to 0.25, being lowest in the clay areas and the highest in the sand and gravel areas (Freeze and Cherry 1979, Kling *et al.* 1993, Korkka-Niemi and Salonen 1996).

Groundwater discharge is mainly into Pyhäjärvi, and also into the cultivated area around the esker through the drainage system. Discharge into Pyhäjärvi is the main process for the natural attenuation of PCE as well. Recharge to an unconfined aquifer composed of sand and gravel can be estimated to be equivalent to at least 60% of the annual rainfall in the esker areas in Southern Finland (Niini and Niini 1995, Korkka-Niemi and Salonen 1996). Estimations of recharge rates outside the coarsest parts of the aquifer were based on the average grain-size distribution of the surficial sediments and the annual rainfall of the area. Resulting recharge rates in the present area vary from 130 mm a⁻¹ to 330 mm a⁻¹. The specific yield of the aquifer can be estimated to be 20%–30% (Freeze and Cherry 1979,

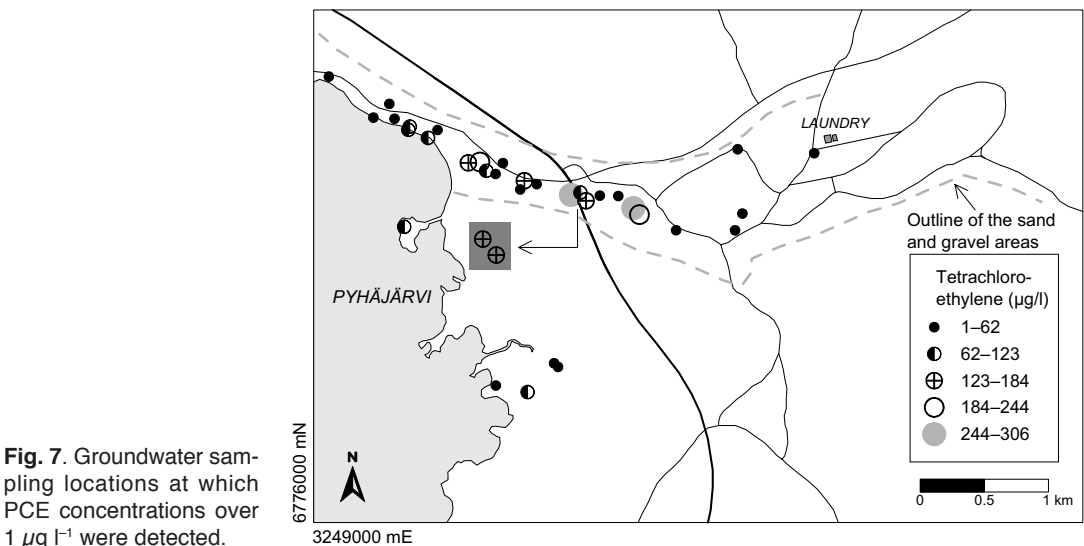


Fig. 7. Groundwater sampling locations at which PCE concentrations over $1 \mu\text{g l}^{-1}$ were detected.

Anderson and Woessner 1992, Korkka-Niemi and Salonen 1996). Specific yield parameter was needed for transient transport simulations.

PCE concentrations of more than $1 \mu\text{g l}^{-1}$ were found in 35 water samples (Table 2 and Fig. 7), together with minor concentrations of TCE. The limit of $1 \mu\text{g l}^{-1}$ was used because there are background concentrations of PCE in the area caused by aerial transport from the dry-cleaning laundry. Normally 99% of PCE is released into atmosphere (Vesi- ja ympäristöhallitus 1994).

Calibrated transmissivity (T) values of the upper model layer are presented in Fig. 8. These values were obtained from MODFLOWP.

The groundwater flow model was capable of creating a groundwater flow pattern and a distribution of hydraulic heads that could be confirmed and measured in the field (Fig. 9 and 10). The groundwater flow connection underneath the clay-covered area was also shown in the model, which verified the validity of the PCE concentrations measured 1.5 kilometres south of the esker (Fig. 10), even though the groundwater flow velocity in this area was highly underestimated in the flow model. This confirms the assumption that all the observed PCE concentrations originate from a single source. The flow connection is caused by the higher hydraulic conductivity zones to the southwest due to the coarse-grained material of the sandy till unit connected with esker sands (Fig. 6). The

coarse-grained material was detected in drill-holes K5, 14, 15 and 16 (Fig. 4).

The concentrations of PCE in 1998 as calculated by the model are displayed in Fig. 11, and the simulated estimates for the natural attenuation of PCE up to the year 2020 are shown in Figs. 12 and 13. According to a statute issued by the Ministry of Social Affairs and Health (effective May 2000), potable water should not contain more than $10 \mu\text{g l}^{-1}$ tetrachloroethylene and trichloroethylene (Anon. 2000). The simulations indicate that this level will be reached by the year 2030 at the latest.

Discussion

The contaminant transport model suffered from scarce input data, as only the source of PCE

Table 2. Measured PCE values (PCE concentrations of more than $1 \mu\text{g l}^{-1}$ in samples).

Parameter	Value
Minimum	$1.1 \mu\text{g l}^{-1}$
Maximum	$305.1 \mu\text{g l}^{-1}$
25%-tile	$10 \mu\text{g l}^{-1}$
75%-tile	$110 \mu\text{g l}^{-1}$
Median	$39.5 \mu\text{g l}^{-1}$
Mean	$76.2 \mu\text{g l}^{-1}$
Standard deviation	78.9

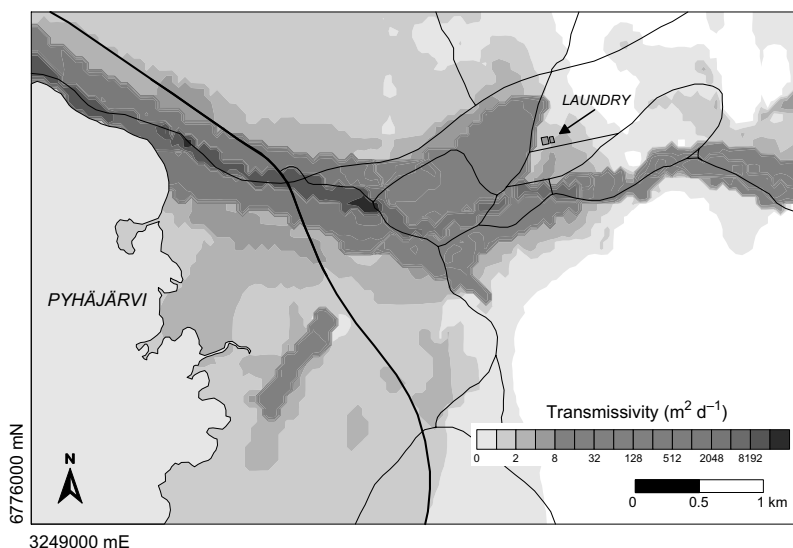


Fig. 8. Calibrated transmissivity values ($\text{m}^2 \text{d}^{-1}$) of the upper layer of the model.

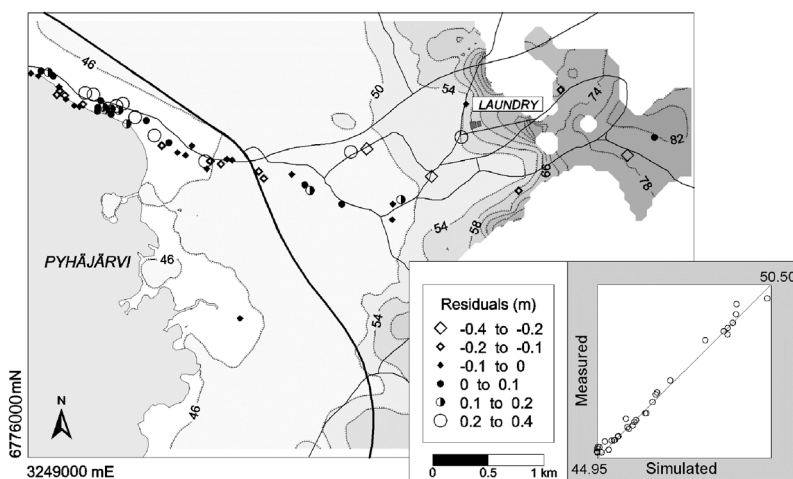


Fig. 9. Residuals and calculated head (m above sea level) in layer 1 of the model. Contour interval is 4 metres. Comparison of measured and simulated heads within the range of 44.95–50.50 metres above sea level is presented in the scatter diagram.

and the measured concentrations in the observation points were known, so that it had to be calibrated to concentrations observed at one point in time (trial-and-error calibration). The spill of PCE could not have happened earlier than in 1963, however, which was when the dry-cleaning laundry was built. In addition, comparison of the measured shape and size of the plume with the maximum time available for solute transport indicated that the ratio of longitudinal to transverse dispersivity (α_L/α_T) in the aquifer must have been more than 8, which can be considered as a reasonable estimate (see e.g.

Zheng and Bennett 1995).

The most severe inconsistency between the flow model and the transport model occurred in the area of the dry-cleaning laundry itself. The observed distribution of hydraulic head did not suggest any major sedimentological heterogeneities in the area, although the transport model required some preferential flowpaths in order to produce the best fit (or even a possible fit). However, recent studies by Zheng and Gorelick (2001) have revealed that the relative preferential flow paths resulting from decimeter-scale aquifer heterogeneities appear to have a

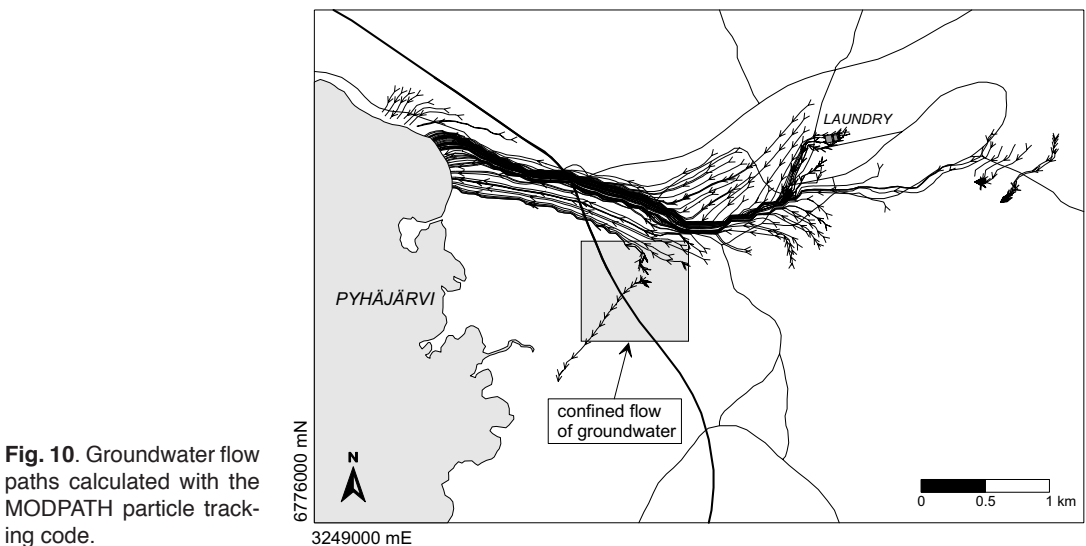


Fig. 10. Groundwater flow paths calculated with the MODPATH particle tracking code.

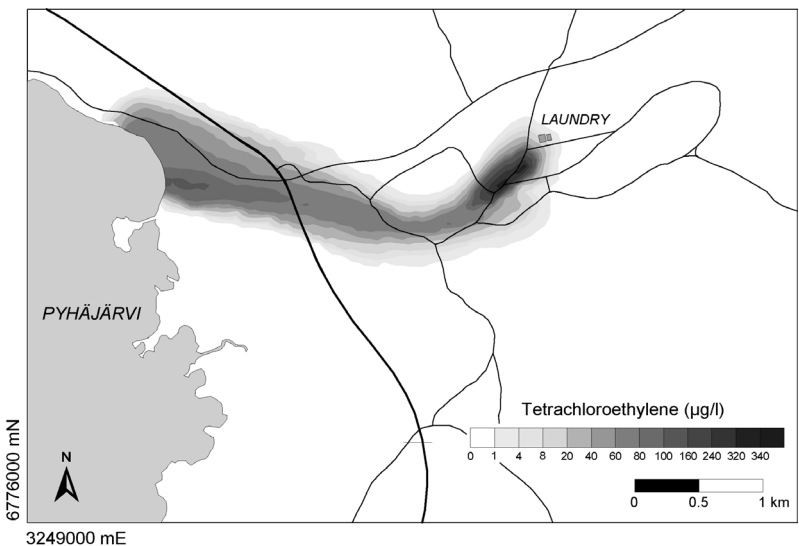


Fig. 11. Concentrations of PCE in 1998 as calculated by the model.

dominant effect on plume-scale transport.

The transmissivity values calibrated for the flow model (Fig. 8) resulted in hydraulic conductivities equal to those of the fine sand and silt in the area of the dry-cleaning laundry, which was also verified by the examination of the exposed surface materials. The final simulations were performed on the assumption that PCE had passed through the preferential flowpaths from the area of the dry-cleaning laundry to the coarser esker material about 250 metres away in two years. The average flowpaths were obtained

from the flow model, and the contaminant was introduced to the transport model in the resulting cells. Without the introduction of preferential flowpaths, the plume would not have reached Pyhäjärvi during the time the dry-cleaning laundry has been operating. This results in a lack of information on PCE concentrations in the area of the dry-cleaning laundry and explains more precisely the distribution of PCE concentrations in the remaining parts of the aquifer, as presented in Fig. 11.

The main road of the area cuts through

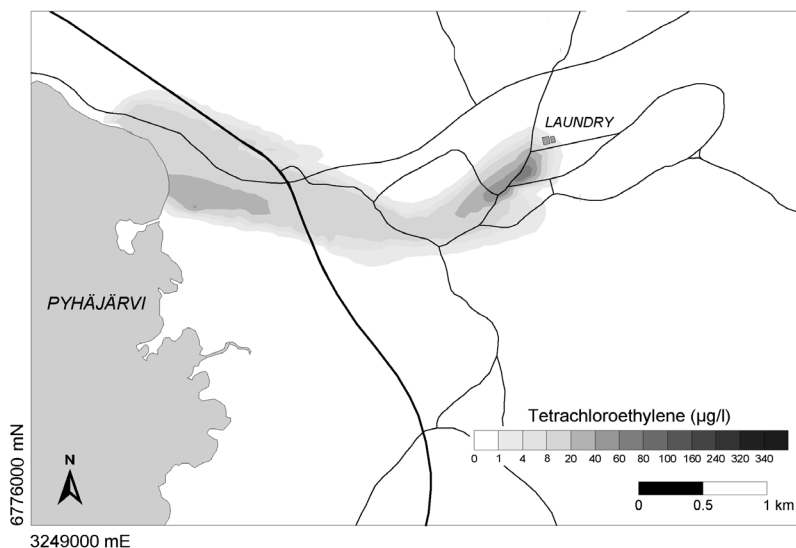


Fig. 12. Concentrations of PCE in the year 2010 as calculated by the model.

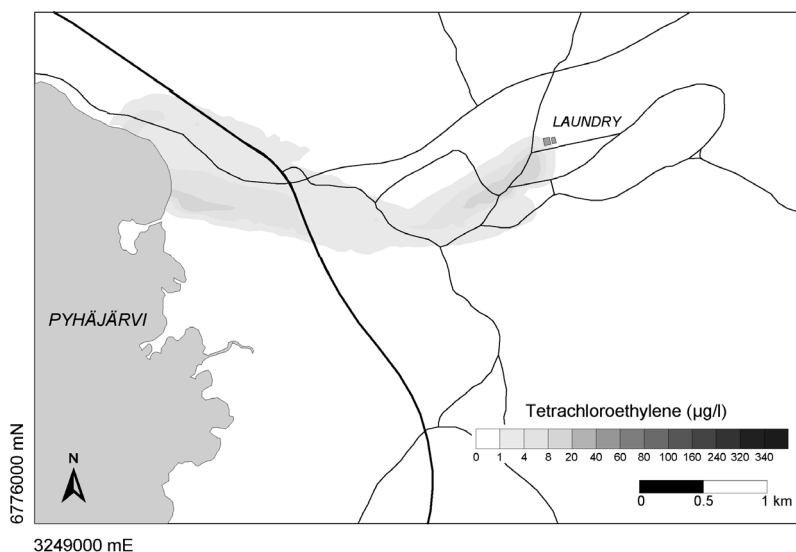


Fig. 13. Concentrations of PCE in the year 2020 as calculated by the model.

the uppermost part of the aquifer and causes minor discharge into the drainage system. This contaminated water has probably polluted two groundwater sampling locations presented in the shaded area in Fig. 7.

The solute transport model failed to generate the observed plume to the southwest underneath the clay-covered area as shown by the particle track on Fig. 10. This is probably caused by structural inexactnesses in the conceptual model in that area.

Groundwater flows southwards beneath the clay area (Fig. 6) under anaerobic conditions, in

which the degradation of PCE results in increasing concentrations of TCE (e.g. Fetter 1993). The ratio of PCE/TCE concentrations was found to be slightly higher in that area.

Conclusions

Suggestions for further investigations into the sedimentological features of the area of the dry-cleaning laundry are recommended. Transport modelling in that area would require more

detailed information and a different approach to constructing the conceptual model, as suggested by Anderson (1989), for example. New information was also obtained from measurements of PCE concentrations in the groundwater of the area of the dry-cleaning laundry at the end of the year 2000. These analyses show that the residual plume predicted for that area by the model exists.

The natural attenuation time of a groundwater constituent depends on how well the source can be managed. If the soil and highly contaminated groundwater in the area of the dry-cleaning laundry could be treated, the attenuation process for the whole aquifer area would be faster. This would require removal of the contaminated soil and treatment of the groundwater with active carbon or oxidation processes. In material with a higher hydraulic conductivity, PCE has been flushed from the soil particles and mixed with a large amount of groundwater. The model suggests that the total amount of contaminated groundwater in glaciogenic material is about 10 400 000 m³, which is far too large a volume to be cleaned up. Most of this amount of water is not greatly contaminated, however, and the remediation costs per unit of PCE removed would be much higher than in the area of the dry-cleaning laundry.

Unfortunately the amount of PCE in the soil and in groundwater near the laundry is not known. The source should be monitored and studied in more detail, so that the simulations would also apply to cases with different source control methods.

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