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Mathematical modelling of groundwater pollution in a small heterogeneous aquifer at Kärkölä, southern Finland

Yhteenveto: Kärkölän likaantuneen pohjavesialueen matemaattinen mallinnus

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CONTENTS

MATHEMATICAL MODELLING OF GROUNDWATER POLLUTION IN A SMALL HETEROGENEOUS AQUIFER AT KÄRKÖLÄ, SOUTHERN FINLAND

Taina Nystén

A two-dimensional finite difference solute transport model MOC is employed here to test the applicability of the groundwater modelling methodology of a small heterogeneous aquifer and to obtain a better understanding of groundwater flow and solute transport in a groundwater area polluted with chlorinated phenols. The area is located on a esker south of the Salpausselkä I zone, and consists of the esker area proper, close to a bedrock depression, a bedrock area lying between them, and the valley of a brook, Pyhäoja. The groundwater in the bedrock depression and the Pyhäoja valley is confined. The polluted groundwater flows from till layers in the bedrock depression down to the sand and gravel layers of the Pyhäoja valley, and concentrations as high as 100 000 μg l^{-1} have been recorded in the area. The currently closed Kukonmäki groundwater intake lies at the intersection of the esker and the Pyhäoja valley.

The groundwater model provides a holistic view of the geology of this heterogeneous aquifer. The fate of a plume of contaminant caused by a single emission in an area between the contamination source and the outflow area was modelled for a period of 12 years. It is obvious that it will take several decades for the aquifer to be purified by the natural groundwater flow. The simulated groundwater heads and the route taken by the contaminated groundwater fit fairly well with measured values, the mean difference between the measured and simulated heads being −0.18 m during the calibration. The error in the mass balance is less than 0.01 % in the flow model and an average of 5 % in the transport simulations.

The MOC model is suitable within certain limits for predicting groundwater flow and the transport of chemicals in heterogeneous aquifers of this kind, and could prove a valuable tool for planning the restoration of polluted groundwater areas by pumping. The results of the modelling can also be used for planning more accurate applications. In principle, a more precise solution could be obtained by using a three-dimensional model, provided that more detailed hydrogeological data were available. In practice, the use of such a model is limited by the lack of suitable methods for monitoring and measuring the properties of an aquifer of this kind, since its success is highly dependent on the available geological data.

1 INTRODUCTION

1.1 Development and application of mathematical groundwater models

Groundwater modelling currently occupies a prominent position in the planning of the use of groundwater and evaluation of the extent of pollution. According to Javandel et al. (1984), numerical methods are required to determine flow conditions in heterogeneous geological formations, and such methods were indeed already in use in the 1960's, but it was not until the 1970's that rapid advances in computer technology enabled the elaboration and introduction of various mathematical models, the use of which then increased markedly in the late 1980's. In addition to flow modelling, the development of groundwater models for porous media has also included heat and chemical transport models (Mercer and Faust 1980b, van der Heijde et al. 1988).

Flow, heat and contaminant transport models (Granlund and Paasonen-Kivekäs 1991, Iihola et al. 1992) were introduced in Finland in the late ·1970's, while the modelling of groundwater in fractured rock was developed later, mainly in the context of nuclear waste disposal (e.g. Meling 1984, Anttila 1985, 1986; Ylinen et al. 1985, Pitkänen and Pirhonen 1987, Suksi et al. 1992, Niemi and Kontio 1993, Niini et al. 1993, Saksa 1993). Two of the largest artificial groundwater projects in Finland rely on modelling techniques, namely that of Turun Seudun Vesi Oy in Virttaankangas and the Utti project implemented by Kymenlaakson Vesi Oy (Laukkanen et al. 1991a, 1991b; Laukkanen and Saijonmaa 1991). Modelling was used at Virttaankangas to determine the location and number of well sites and infiltration areas so as to ensure that these would correspond in an optimal manner to the water extraction requirements. The application of solute transport models to porous media commenced in the 1980's, e.g. for the modelling of groundwater flow and chloride transport at the Terrisuo waste landfill area in Tuusula (Ahlberg and Soveri 1988, 1991).

The MOC (Method of Characteristics) model has been used extensively in Denmark and Sweden (e.g. Engesgaard 1988, Van Rooy et al. 1988, Destouni et al. 1991, Henriksen et al. 1991, Jensen 1991), and has been employed in Finland e.g. at Virttaankangas in the districts of Alastaro and Oripää, at Terrisuo in Tuusula, at Hyrylä, at Järvelä in Kärkölä (Nystén 1993) and in the Joutsenonkangas area in the districts of Lappeenranta and Joutseno. The work being carried out at Hyrylä is focused on modelling the transport of contaminants from an industrial area and a refuse disposal site, and the results obtained have been used to draw up a groundwater protection plan (Granlund et al. 1993, Suomela et al. 1993). The National Road Administration in Finland is currently funding a research programme concerned with the effects of salting of the roads on the groundwater, ˙employing models to describe the transport of road salt in the groundwater at two sites, one of which is Joutsenonkangas. The main objective of this part of the work was to use the MOC model to predict future concentrations of chloride in the Joutsenonkangas aquifer (de Coster et al. 1993). It will be possible to use the results obtained from this aquifer as a guideline when evaluating the effects of road salting and future trends in chloride migration and its concentrations in aquifers of this type.

1.2 The polluted groundwater area at Kärkölä

The sawmill situated at Järvelä in the municipality of Kärkölä (Fig. 1) in southern Finland manufactures plywood, chipboard and sawn timber. The company began to use Ky5 as a fungicide to prevent blue staining in the 1930's, discontinued it in 1984, when the product was taken off the market, and is currently using Kemtox S10 for that purpose. The sawmill was destroyed by fire in 1976 and a new building was constructed on the same site, the new irrigation basin being located close to the former Ky5 impregnation site which had been destroyed by fire. The compound Ky5, a total of 7 000–10 000 kg of which was used for wood preservation annually (Nystén 1988, 1989, 1990, 1991a, 1991b), is composed of tetra-, penta- and trichlorophenols and is classified as Class I toxic substance.

The Kukonmäki groundwater intake was found to be polluted in 1987. Measures were
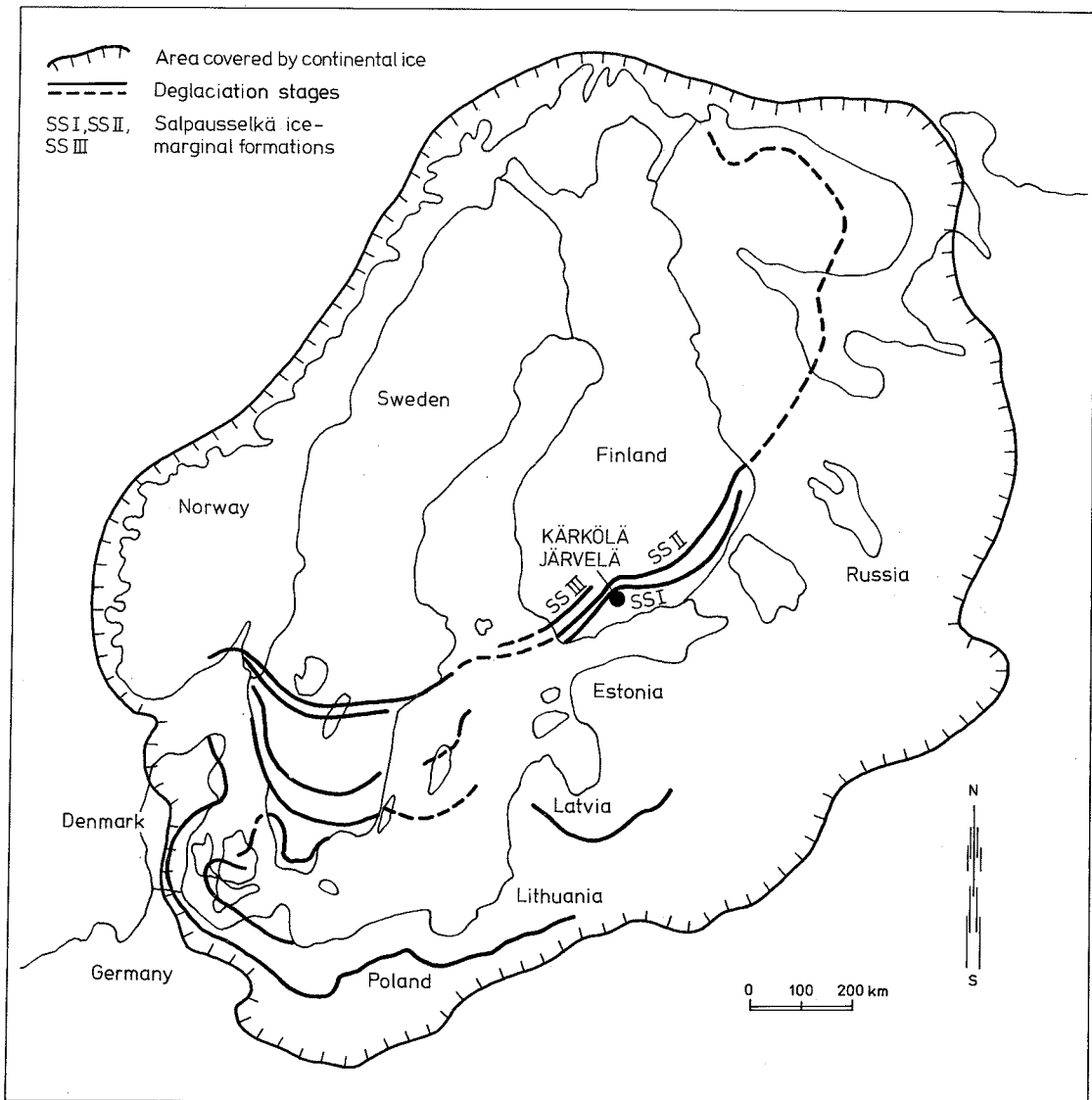
Fig. 1. The extent of ice sheet during the last glaciation and location of the area studied at Järvelä in the municipality of Kärkölä in southern Finland (Haavisto 1983).

initiated as soon as the extent of the pollution at Kärkölä was discovered to find purification methods which could be used to remove the chlorinated phenols from the groundwater. Well site investigations were performed there in spring 1990 to examine the possibilities of pumping out the polluted groundwater (Insinööritoimisto Paavo Ristola Oy 1990). Ettala and Koskela (1992) studied treatment of this polluted groundwater at a biological municipal sewage treatment plant, and tests were carried out with a microbiological method (Valo 1990, 1991, Valo and Hakulinen 1990) and aerobic fluidized bed reactors (Puhakka and Järvinen 1992). Work on the restoration of the polluted groundwater area commenced during 1993.

1.3 Aim of the investigation

This paper discusses the modelling methodology and its basic geological criteria. The applicability of the MOC model was tested with respect to flow and transport modelling in the case of a small heterogeneous aquifer. The principal emphasis in the model application is on the geological investigation of the area. An explanation is also given of the types of geological data employed in the application of the MOC model, and results are presented which could be applied to the restoration of the groundwater area, for example.

2 Groundwater modelling

2.1 Groundwater models

Modelling can be used as a practical tool when planning the pumping of groundwater. The necessary source data can be acquired through field tests and measurements and the models are used to account for the flow and quality of the groundwater and contaminant and heat transport. The use of such a model requires a knowledge of the scientific principles connected with the research problem, the mathematical methods to be used and the geology of the area to be examined (Mercer and Faust 1980a, van der Heijde et al. 1988). Groundwater modelling programs have been described extensively in the literature, and these are classified according to their capabilities in a database compiled e.g. by the International Groundwater Modelling Center (IGWMC). The usability and reliability of such models are also evaluated in the database (van der Heijde et al. 1988). The applicability of a model for the solution of the problems concerned should be verified upon selection, its usability being dependent on the technical properties of the program, e.g. its structure, documentation and adaptability. A model can be considered reliable if the descriptions contained in it can be justified scientifically and it has been tested (verified and validated) under field conditions (e.g. Mercer and Faust 1980a, EPRI 1988, van der Heijde et al. 1988). The modelling of groundwater areas involves the combining of research data in order to facilitate the evaluation of existing information and gain the advantages of being able to assess the level of uncertainty of the modelling process.

The most common groundwater models employed in Finland are flow models for water supply. Other predictive models traditionally employed when solving groundwater problems are chemical and heat transport models and geochemical and deformation models. An increasing number of application opportunities can be expected to open up for the constantly developing technique of predictive modelling as a tool in groundwater investigations and planning.

Identification models are used to estimate the physical parameters of an aquifer, e.g. its hydraulic conductivity and storage coefficient, given source data that consist of known properties of the aquifer. The simplest method of determining such physical parameters is subjective trial and error (Bear 1979).

Optimization models are used (1) to identify aspects of a problem which require more detailed research, and the resulting information is transferred to groundwater flow or transport models. Optimization models are used (2) to determine the amount and type of source data required for the solution of groundwater problems and (3) to specify the type of information required to explore the flow field and the optimal density of the observation grid and monitoring program at the initial stage in the fieldwork. Further advantages include the opportunity to make preliminary surveys of areas where it is impossible to perform fieldwork for reasons of cost etc. (van der Heijde et al. 1988). This was the case with the polluted groundwater area at Kärkölä, where it was impossible to establish an investigation network with regular intervals that would cover the entire area.

Models can be used as an aid to planning and decision-making, for risk assessment and in the case of legal proceedings. Research of this type can reduce costs, optimize technical solutions and maximize the supply of groundwater and its storage in the ground. Models can also be used to facilitate the planning of restoration measures in the case of polluted groundwater areas. Features modelled in this study include the effects of pumping of the contaminated groundwater on groundwater flow in the aquifer. Model calculations can be used as a basis for drawing up

protection plans for groundwater areas, and it is also possible to use modelling to determine the transport velocities and directions of contaminants, to determine their dilutions and to outline protective measures to prevent them from spreading further. It is pointed out by Anderson and Woessner (1992), however, that although it is likely that hundreds of predictive models have been constructed since the 1960's, only four post-audits are reported in the literature, which suggests that such models are traditionally used in a 'crisis mode' rather than a 'management mode'.

2.2 Groundwater model development needs

It is difficult to examine the heterogeneity of a groundwater area and its effects. According to Konikow (1991), mean values for its hydraulic properties are not in themselves sufficient for groundwater modelling, but variances and correlations will also be required in future models. In addition, more attention should be paid to field measurement techniques and to the role of conceptual models. Concentration, hydraulic conductivity and effective porosity are often presented as uniform properties of a given sub-area in the three-dimensional modelling of chemical transport, for example, and in practice these quantities are measured on a finite scale which may be different for each of the properties. The comparability of the results obtained is also dependent on the measurement techniques and sampling depths. More and more extensive sand-box laboratory tests are required to examine heterogeneity and anisotropy, on account of the existence of uncertainty factors even in the most accurate field measurements (Rushton 1989, Konikow 1991).

The properties of contaminants may affect the groundwater velocity, while that of a non-reactive solution in a porous medium is dependent on advection and dispersion. Uncertainty about the true flow velocity and distribution of contaminant concentrations is compensated for in practice by the use of a dispersion coefficient when calibrating the model. If transient changes in the flow field and contaminant source are not explicitly accounted for by advection, then their effect will be induced an apparently greater dispersion than actually exists. The more accurately groundwater flow velocities and solute concentrations can be defined, the more exact will be the definition of the apparent magnitude of dispersivity and the calibration of the model (Rushton 1989, Konikow 1991).

Information on dispersion in a porous anisotropic medium is still poorly available. It is generally defined in terms of longitudinal and transverse dispersion, the exact definition of which is usually difficult. Reliable description may well require more than two parameters. Even though hydraulic conductivity may be recognized as an anisotropic property, dispersion is still assumed to be isotropic. Results obtained from sand-box experiments have indicated that longitudinal dispersion in an anisotropic porous medium is dependent on the directions of the flows and that the relation between the hydraulic and dispersive anisotropies is not always consistent, i.e., higher longitudinal dispersion is not always aligned with the same axis of the hydraulic conductivity tensor but instead depends on the nature and scale of the geological factors causing the hydraulic anisotropy (Konikow 1991).

If the solutes being transported are reactive, practical problems may arise in handling the situation, as groundwater modelling traditionally either has been geochemical, in which reactions are the primary mode of control, or has involved the modelling of flows and transport. Attempts have been made in the last few years to couple geochemical and transport modelling (Appelo and Willemsen 1987, Bütow et al. 1989, 1990; Courain-Ribstein et al. 1989, van Meurs et al. 1989, Read and Liew 1989, Sauty 1989, Taat et al. 1989, Jensen 1991, Pitkänen and Pirhonen 1991). Mathematical problems arise when the reaction terms are markedly non-linear, numerous chemicals in the solution have a profound effect on the concentration in the solution or the solution being modelled reacts with a solid phase. It is difficult to describe mathematically a precipitation dissolution reaction taking place in a transported solute, but it may significantly alter the hydraulic properties of a porous medium. There is seldom adequate information on the types and rates of reactions for specific solutes or on the mineral composition of the area concerned,

the latter of which may vary significantly. Further research is required in order to examine the effect of mineralogy on transport. It may be difficult to describe chemical reactions in mathematical formulations, and these should certainly be developed further in order to account for complex reactions which take place during the transport of pollutants. The description of the transport of immiscible or partly miscible contaminants such as many organic chemicals calls for the recognition of additional processes and parameters. Multiphase modelling may be required to represent phase compositions, inter-phase mass transfer, and capillarity, but no well-documented multi-dimensional and efficient multiphase models are yet available which are applicable to the contamination of groundwater by immiscible organic chemicals. Research into organic chemicals in groundwater has nevertheless yielded information on the significance of microbiological processes in transforming and degrading these contaminants, and such results can be exploited for the microbiological restoration of contaminated aquifers (Konikow 1991).

2.3 Theory of groundwater flow modelling

2.3.1 Hydraulic conductivity

Groundwater flow in a fully saturated zone can be described by means of Darcy's law as first put forward in 1856, and this can be extended to apply to three-dimensional flows (e.g. Bear and Verruijt 1987). The coefficient K appearing in Darcy's law stands for hydraulic conductivity, which is dependent on the properties of the solid medium and the flowing liquid. It is a scalar $(L\ T^{-1})$ which expresses the ease with which a fluid is transported through a tortuous void space. Hydraulic conductivity is primarily attributable to the structure of the porous medium, i.e. the nature of the connections in the void space. The most relevant solid matrix properties are grain and pore size distribution, shape of the grains and pores, tortuosity, specific surface, and porosity (Frank and Kleber 1966). Hydraulic conductivity in till is determined in particular by the proportion of fines.

Hydraulic conductivity K can be expressed as

$$K = k \cdot \rho \cdot g \cdot \eta^{-1} \qquad (1)$$

where

k is permeability of the porous medium),
ρ is the density of fluid,
g is the acceleration of gravity and
η is viscosity of fluid (e.g. Bear and Verruijt 1987).

The permeability of an aquifer can be evaluated in terms of soil type and hydraulic conductivity (K), the latter of which can be determined in the laboratories or from flow velocity and permeability measurements performed in observation tubes (Mälkki 1978, 1979; de Marsily 1986, Bear and Verruijt 1987). Major fluctuations are observed in the hydraulic conductivity of the various soils (Fig. 2), and
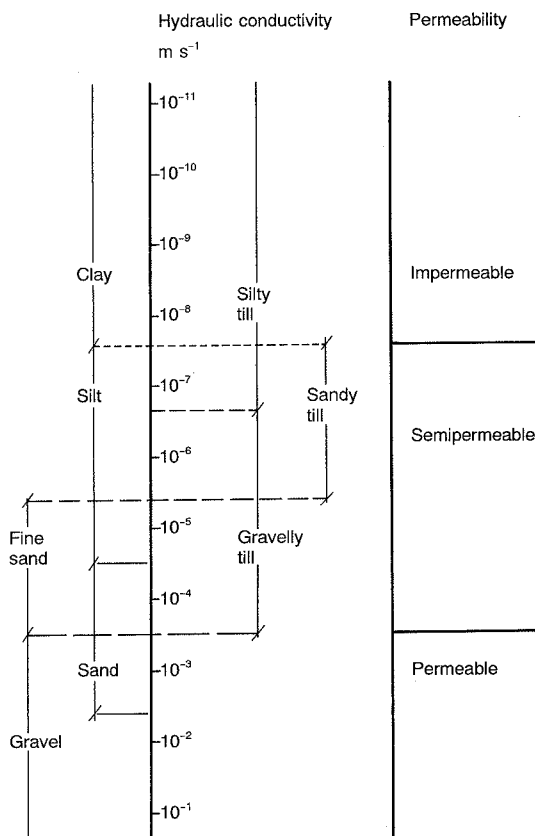

Fig. 2. Typical values for hydraulic conductivity and permeability (modified from Hatva 1985). Soil material according to the Geo classification (used in Finland only).

examples of such values are presented by authors such as Knutsson and Morfeldt (1973), Airaksinen (1978), Mälkki (1979), Freeze and Cherry (1979, p. 28–29), Hatva (1985, p. 58), RIL (1985, p. 420), de Marsily (1986, p. 78) and Anderson and Woessner (1992, p. 40). Transmissivity (T) as a soil permeability property is defined as

$$T = K \cdot b \qquad (2)$$

where b is the thickness of the aquifer.

2.3.2 Mathematical description of flow in a porous medium

The mathematical description of groundwater flow is based on Darcy's law and the law of mass conservation. A more detailed derivation of the groundwater flow equations used in this section is presented elsewhere, e.g. in another publication on the geology and mathematical modelling of polluted groundwater in Kärkölä (Nystén 1993). In the case of a steady flow the three-dimensional equation (x,y,z) for groundwater flow in an anisotropic porous medium can be written as

$$K_x \frac{\delta^2 \phi}{\delta x^2} + K_y \frac{\delta^2 \phi}{\delta y^2} + K_z \frac{\delta^2 \phi}{\delta z^2} = 0 \qquad (3)$$

where

K_x, K_y, K_z are hydraulic conductivities in the direction of the axes x, y and z and
ϕ is hydraulic head.

If porous medium is isotropic ($K_x = K_y = K_z$), the equation (3) for steady-state flow may be inserted into Laplace's equation:

$$\frac{\delta^2 \phi}{\delta x^2} + \frac{\delta^2 \phi}{\delta y^2} + \frac{\delta^2 \phi}{\delta z^2} = \nabla^2 \phi = 0 \qquad (4)$$

The processing of a stationary flow of this kind requires knowledge of the distribution of hydraulic conductivity in the area and either the hydraulic head or the normal component of flow velocity at its boundaries. The examination of a

transient flow first requires determination of the compressibility of the porous medium and the liquid. The following equation can be given for transient flow in an isotropic, homogeneous medium:

$$\frac{\delta^2 \phi}{\delta x^2} + \frac{\delta^2 \phi}{\delta y^2} + \frac{\delta^2 \phi}{\delta z^2} = \nabla^2 \phi = \frac{S_s}{K} \frac{\delta \phi}{\delta t} \qquad (5)$$

where S_s is the specific storage coefficient (e.g. Saari et al. 1984, p. 29). The equation can also be used for phreatic aquifers provided that the fluctuations in the thickness of the water-saturated layer are relatively small (e.g. Airaksinen 1978).

2.3.3 Hydraulic approach to flow in aquifers

Flow through a porous medium usually takes place in a three-dimensional manner. According to Bachmat et al. (1980) and van der Heijde et al. (1988), however, the most common flow models are two-dimensional, enabling the examination of flow in phreatic or confined aquifers.

Since the geometry of most aquifers is such that they are thin relative to their horizontal dimensions, it is possible to introduce a simpler approach in which it is assumed that the flow is essentially horizontal throughout the aquifer or that it may be approximated as such, neglecting any vertical flow components. This is strictly true for flow in a horizontal, homogeneous, isotropic, confined aquifer of constant thickness and with fully penetrating wells, and a good approximation is still achieved if the aquifer thickness varies but in such a way that the variations are much smaller than the average thickness (Bear 1979, p. 26–28).

The assumption regarding an essentially horizontal flow does not hold good for regions in which the flow is characterized by large vertical components, as in the vicinity of partially penetrating wells, or outlets in the form of springs, rivers, dug pits, etc. A simple rule of thumb is that the flow is three-dimensional at a distance of less than 1.5 to 2 times the thickness of the aquifer (Bear 1979, p. 27–28).

The above assumption is also applicable to leaky aquifers. When the hydraulic conductivity of the aquifer is much larger than that of the

semi-permeable layer and the thickness of the former much greater than that of the latter, the flow in the aquifer is essentially horizontal, but that in the semipermeable layer is essentially vertical (Bear 1979, p. 27–28).

The approximation that takes the flow to be essentially horizontal in phreatic aquifers constitutes the basis for Dupuit's assumption that a three-dimensional flow field can be reduced to a two-dimensional one by assuming that the flow is solely horizontal. The magnitude of the hydraulic gradient is taken to correspond to the gradient of the groundwater table in a phreatic aquifer and not to change as a function depth (Bear 1979), but there are also models, such as UNSAT 2, in which Dupuit's approximation is not employed and which enable fluctuations in hydraulic head to be examined as a function of depth (van der Heijde et al. 1988).

2.3.4 Initial and boundary conditions

In order to obtain a unique solution for a partial differential equation corresponding to a given physical process, additional information about the physical state of that process is required. This information is described by boundary and initial conditions. Mathematically, boundary conditions include the geometry of the boundary and the values of the dependent variable or its derivative normal to the boundary. To obtain a solution to such an equation, information is required about the properties of the aquifer which affect groundwater flow, e.g. the geometry of the domain, physical coefficients and also groundwater flow and heat or solute transport through and at the boundary (Bear 1979, Mercer and Faust 1980b).

Steady-state problems require only boundary conditions, whereas for transient problems it is also necessary to define the initial conditions, i.e., the value of the hydraulic head at all points in the domain for (t=0). According to de Marsily (1986), there are three principal types of boundary condition: prescribed head boundaries, known as Dirichlet's conditions, prescribed flux boundaries, known as Neumann's conditions, and prescribed head-dependent flux boundaries, known Fourier's conditions, although a fourth type can also be recognised: the conditions on a free surface face or on a seepage face, which are

double boundary conditions (de Marsily 1986).

Under Dirichlet's conditions, constituting a boundary value problem of the first type, the hydraulic head is prescribed for all points on this boundary (Bear 1979). This is generally the case where there is contact between the aquifer and a free expanse of water, e.g. a sea, lake or river. The hydraulic head is constant along the aquifer-river contact area (A) and is determined imposed by the water level in the river (Fig. 3), which can recharge or drain the aquifer. An outlet of an aquifer (line of springs) may also be regarded as a prescribed head boundary (de Marsily 1986).

In the second type of boundary value problem, following in Neumann's conditions, the flux normal to the boundary surface is prescribed for all points (Bear 1979). No-flow boundaries include the contact between an aquifer formation and an impermeable layer, a confining bed or unweathered outcrop. Boundaries with a prescribed non-zero flux include wells and ditches (Fig. 4) (de Marsily 1986). In this modelling of the Kärkölä case the boundaries are of the constant head or impermeable type.

Under Fourier's conditions there is a stream draining (or feeding) a water table aquifer but with a layer of low permeability deposited on its bottom (Fig. 5). The difference in hydraulic head across the low permeability $(h_s - h)$ layer creates the necessary gradient for a certain flow (q) per unit surface area of contact between the aquifer and the stream, in accordance with Darcy's law. Thus the flow can be expressed by the equation (6)

$$q = K'[(h_s - h)/\acute{e}] \qquad (6)$$

where

q   is the flow rate or flow per unit surface area of the contact between the aquifer and stream;
K'   is the hydraulic conductivity of the low permeability layer;
h_s is stream head;
h   is aquifer head; and
é   is the thickness of the low permeability layer (de Marsily 1986).

Bear (1979) assigns this type of boundary, when the two domains are separated by a relatively thin semi-pervious layer, to the third type of boundary,
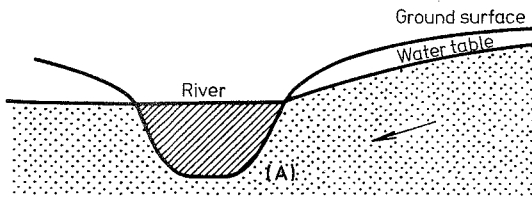
Fig. 3. An example of Dirichlet's conditions. A river as a prescribed head boundary condition (de Marsily 1986).
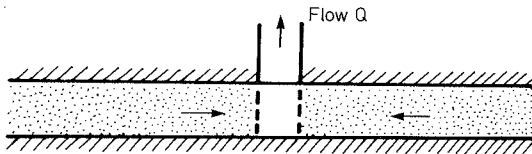

Fig. 4. An example of Neumann's conditions. Prescribed flux (Q) in a well or ditch (de Marsily 1986).
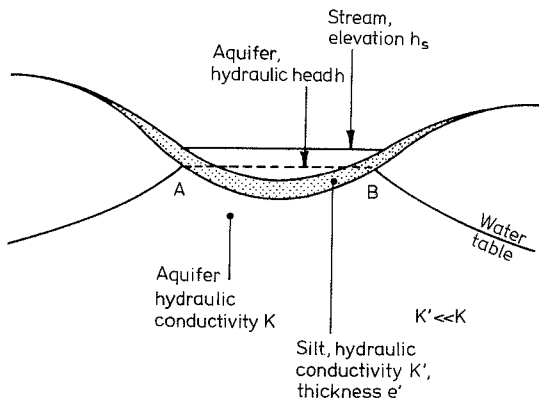

Fig. 5. Fourier's condition between an aquifer and a stream (de Marsily 1986).

corresponding to a mixed boundary condition or Cauchy's conditions.

The most common free surface boundary (phreatic surface) is the water table itself, which is a boundary surface between the saturated flow field and the atmosphere. Atmospheric pressure prevails at this boundary, and a second important characteristic is that its position is not fixed; it may rise and fall with time. Because of the inherent difficulty in modelling ground water systems with free surface boundaries, representation of such a system can sometimes be facilitated with the help of the set of simplifying

assumptions proposed by Dupuit in the 19th century (Franke et al. 1984).

A seepage surface is a boundary between the saturated flow field and the atmosphere along which groundwater discharges, either by evaporation or by moving "downhill" along the land surface in a thin film in response to gravity. An example of a seepage face is represented by the line BC in Fig. 6 (Franke et al. 1984).

2.3.5 Solution methods

The available groundwater models can be classified according to their solution methods into physical, analogue, analytical and numerical types, as suggested by Prickett (1979). Physical models are scale-models which aim at describing the original situation. They have been used since the discovery of Darcy's law and constitute a practicable tool for examining groundwater quality and pollution. Sand-box tests constitute one example of a physical model (Prickett 1979).

Analogue models use some other physical phenomenon or the same phenomenon in some other area to depict the groundwater flow, the most common applications being electrical analogues. Analogue models were primarily used in the 1950's and 1960's, but are less common nowadays (Prickett 1979).
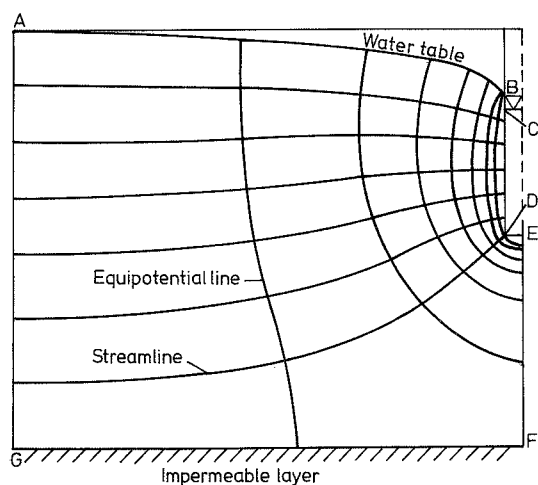

Fig. 6. Flow pattern near a discharging well in an unconfined aquifer. The surface BC forms the boundary condition for an aquifer (Franke et al. 1984).

Concepts of the
physical system

Translate to

Partial differential equation,
boundary and initial
conditions

Finite element
approach

Finite difference
approach

Subdivide region
into a grid and
apply finite
difference approx--
imations to space
and time derivatives

Transform to

Integral equation

Subdivide region
into elements
and integrate

First–order differential
equations

Apply finite difference
approximation to
time derivative

System of algebraic
equations
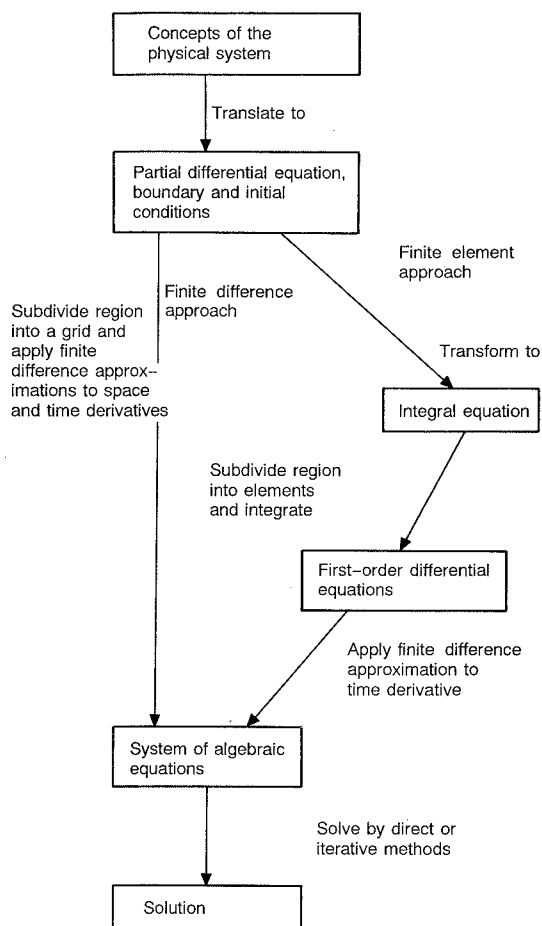
Solve by direct or
iterative methods

Solution

Fig. 7. Generalized scheme for the use of the finite difference and finite element methods (Faust and Mercer 1980).

Analytical models describe groundwater flow by means of partial differential equations which can be solved for cases of simple flow under homogeneous, isotropic conditions. It is often possible to solve equations derived from pumping tests in an analytical manner. Analytical models are easy to use but cannot be solved for the complex flow situations which arise if the area to be modelled has irregularly shaped boundaries and fluctuating flow conditions. Similarly, factors which affect the water balance in the area, such as fluctuations in recharge or pumping, cannot be taken into consideration. Analytic models can sometimes be used as an aid when evaluating the results of a numerical solution (Prickett 1979, Mercer and Faust 1980a, EPRI 1988).

A numerical groundwater model is one in which flow equations are solved numerically to give approximative results. The calculations are based on partial differential equations which are replaced by approximations which are easier to solve. The method can be used for complex situations, such as cases in which the boundaries of the area to be modelled are irregular in shape, the medium is heterogeneous or variations occur in factors affecting water balance in the area, such as recharge or pumping (Faust and Mercer 1980). The use of numerical methods increased in Finland in the 1980's, the most significant of them being the Finite Difference Method (FDM), the Integrated Finite Difference Method (IFDM) and the Finite Element Method (FEM) (Fig. 7) (Bear and Verruijt 1987).

When using the FDM to solve a partial differential equation, a grid is first established throughout the region of interest. For two-dimensional, areal problems, a grid system is overlaid on a map view of the aquifer. There are two common types of grid, mesh-centred and block-centred (Fig. 8). A mesh-centred grid is convenient for problems in which values for the head are specified at the boundary, whereas a
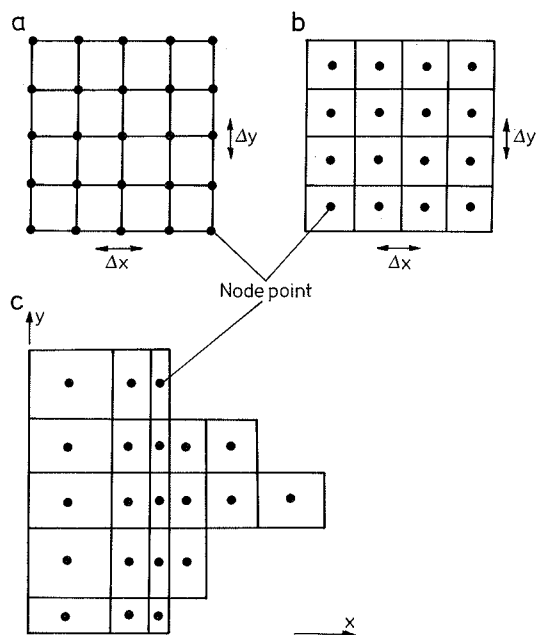
Fig. 8. Grid systems for two-dimensional, areal problems: (a) grid of mesh-centred nodes, (b) block-centred nodes and (c) irregular grid (Faust and Mercer 1980).

block-centred grid has an advantage in the case of problems where the flux across the boundary is specified. The differences between the two types are nevertheless minor from a practical point of view. The IFDM is a special form of FDM which employs an arbitrary grid (Faust and Mercer 1980).

While the FDM approximates differential equations by a differential approach, the FEM adopts an integral approach. The term FEM actually refers to the numerical method by which a region is divided into subregions called elements, of a shape determined by a set of points known as nodes (Fig. 9) (Faust and Mercer 1980).

The finite element method is more flexible than the finite difference method, especially since, when dealing with heterogeneous and anisotropic cases, it allows elements of the desired sizes and shape to be formed by following the appropriate surfaces (Bear and Verruijt 1987, p. 222). Bear and Verruijt (1987) note, however, that variants of the finite difference method exist which are very similar to the finite element method (e.g. integrated finite difference). Thus the two methods may be considered more or less equivalent. Akkanen (1988) regards that the boundary conditions can be set more easily and more accurately in the finite element method than in the finite difference method.

2.4 Application of the model

The stages involved in groundwater modelling are initialization of the problem, material preparation, model calibration and problem solving (Fig. 10). Groundwater information is collected and the aims are set at the beginning of the modelling stage. A conceptual model is created of the area which contains information on its geology and factors which contribute to its water reserves and quality. The aims of the modelling are set at this point, and a preliminary decision is taken regarding the objectives of the modelling and the type of model required (Mercer and Faust 1980a, EPRI 1988, van der Heijde et al. 1988).

The boundaries of the area to be examined are determined as accurately as possible on the basis of its geology to form a FDM grid or a FEM
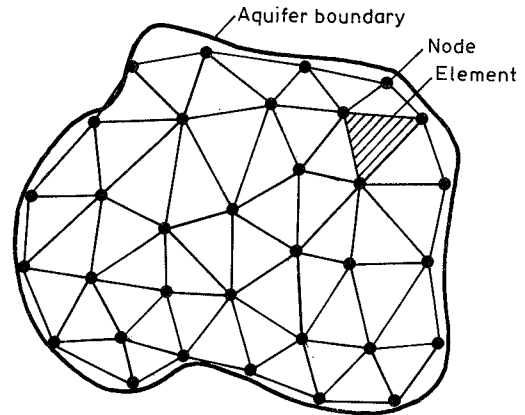

Fig. 9. A finite element configuration showing a typical node and element (Faust and Mercer 1980).
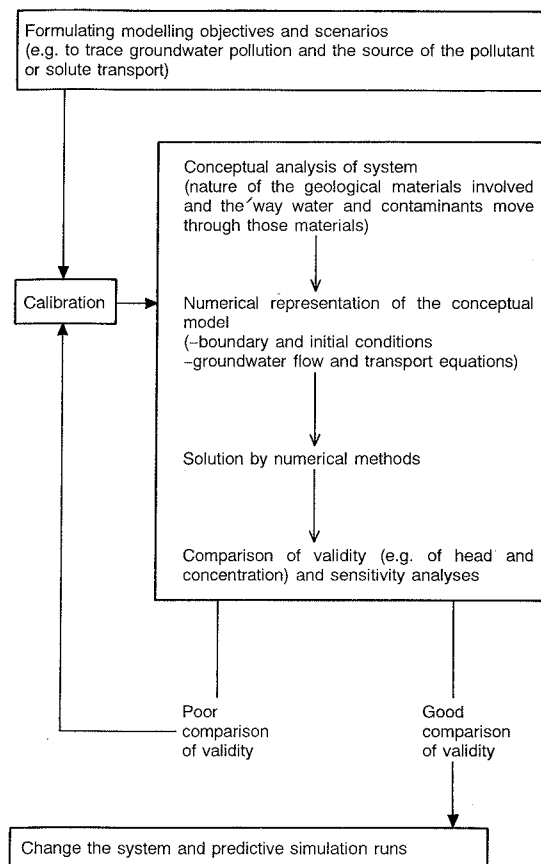

Fig. 10. Flow diagram for flow and transport modelling (according to EPRI 1988 and van der Heijde et al. 1988).
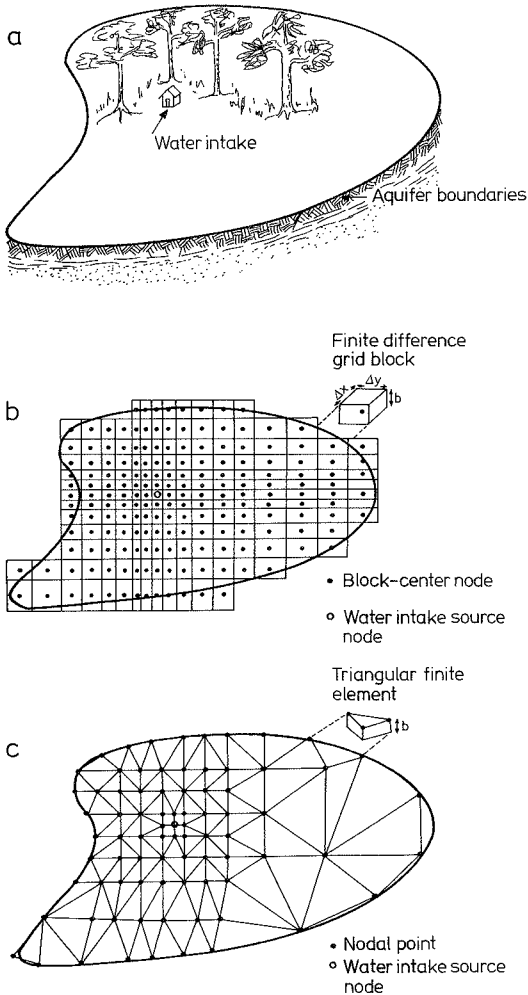
a

Water intake

Aquifer boundaries

Finite difference
grid block

b

Δy

b

• Block–center node

○ Water intake source
node

Triangular finite
element

b

c

• Nodal point
○ Water intake source
node

Fig. 11. a) Map of an aquifer showing water intake, b) finite difference grid and c) finite element configuration, where Δx is the spacing in the direction x, Δy is the spacing in the direction y and b is the thickness of the aquifer (modified from Mercer and Faust 1980a).

element network (Fig. 11). Restrictions may exist in the models regarding size of the grid (see the MOC model, section 4.3.2), for example, and the time intervals employed in the actual calculations. Attention is paid to determining the boundaries of the aquifer, and the area is subdivided by means of a grid. Once the grid has been designed, it is necessary to specify the aquifer parameters and initial data, e.g. hydraulic conductivity, thicknesses of the strata and flow in and out of the aquifer.

According to Woessner and Anderson (1992),

calibration targets should be stated before calibration begins. Calibration of a groundwater model involves the calculation of hydraulic heads or pollutant concentrations for comparison with the observed values, in addition to which the boundaries and the water balance of the model is checked. The hydraulic parameters evaluated on the basis of the investigations, e.g. hydraulic conductivity, storage coefficient and dispersivity, are taken to serve as the initial estimates in the calibration, and thus calibration of the model consists of the iterative determination of these parameters and boundary conditions, adjusting the descriptions of the modelled area and the model parameters until the results obtained from the model-based calculations correspond to the measured ones (Mercer and Faust 1980a, Anderson and Woessner 1992). This calibration can be performed either by trial and error or by an automatic procedure. The diagrams in Fig. 12 indicate the stages in both these methods, the

Start

initial parameter estimates
model specification

Run model

update model parameter estimates

Compare
calculated &
observed
values

bad

good

Stop

TRIAL AND ERROR

Start

initial parameter
estimates

Model
specification

Run model

automatic part

calculate new
parameters

Calculate
criteria

no

yes   convergence?

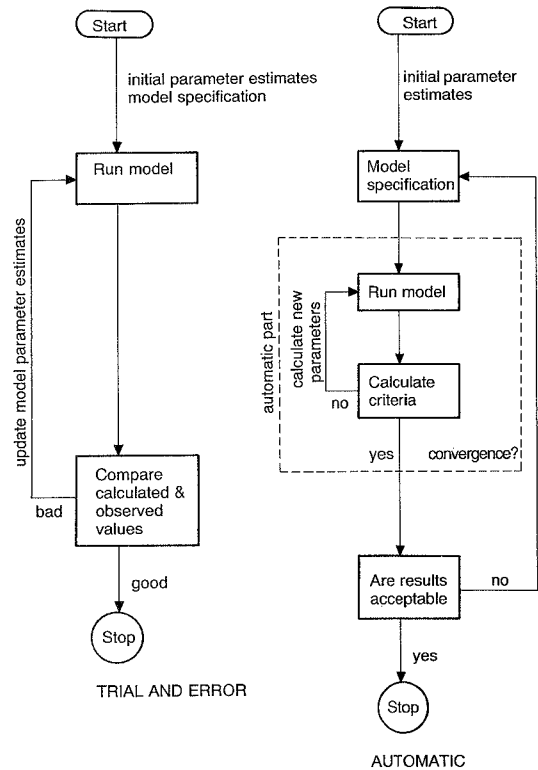Are results
acceptable

no

yes

Stop

AUTOMATIC

Fig. 12. History matching/calibration by trial and error or automatic procedures (after Mercer and Faust 1981, in van der Heijde et al. 1988).

former of which is subjective and slow while the latter requires access to a suitable computer program. Sensitivity runs are performed to assist in the calibration procedure (van der Heijde et al. 1988, Anderson and Woessner 1992).

Once the calibration stage has been completed satisfactorily, one can proceed to the scenario analysis stage. The model can be used to calculate the effect of pumping on the groundwater system and to determine chemical transport in the groundwater and define protection zones. Inaccuracies may occur in the modelling results if the initial data are available in inadequate quantities or are erratic. Examination of the results involves evaluation of their reliability. The use of sensitivity analysis at this stage in the modelling process, for example, provides an insight into the reliability of the computer predictions (Mercer and Faust 1980a, EPRI 1988, van der Heijde et al. 1988, Carrera et al. 1989, Anderson and Woessner 1992).

2.5 Data requirements

Groundwater modelling involves collecting and specifying initial data in connection with initialization of the problem, preparation of the data and calibration of the model. The aims are set and the level of complexity decided upon in conjunction with the formulation of the conceptual model. Proposals regarding the construction of a conceptual model and the design of a grid for each type of aquifer are made by Anderson and Woessner (1992), for example. Modelling may be either regional or local, in addition to which the geology of the area affects to the quantity of initial data required and the heterogeneity of the soil and bedrock constitute a further factor influencing the accuracy of the model. Any inaccuracies arising from complex geology can be reduced by increasing the field investigations and using a denser grid. It is inevitable that uncertainties exist in the boundary conditions and properties of aquifers in spite of the large amount of information available (Konikow 1991), and it is often necessary to redefine the aims in the course of the actual modelling process (van der Heijde 1988).

The source data available are usually insufficient and have often been collected before the actual modelling has commenced, and should thus be filled out by means of field investigations, laboratory tests, parameters quoted in the literature, or estimates if no measurements exist or can be obtained. Any initial estimates should be checked by calibration before inclusion in the final source data. It is important at this subjective modelling stage that the modeller should be in possession of the basic hydrogeological information. The initial data can be used more effectively both by stochastic means such as stochastic partial differential equations, e.g. Monte Carlo simulation, and by geostatistical methods such as kriging (de Marsily 1986, Bouma and Wosten 1987, Peck et al. 1988, Ree et al. 1989, Kovar 1990, Anderson and Woessner 1992). Peck et al. (1988) recognise three categories of flow parameter estimation: the direct approach, the indirect approach and the geostatistical approach.

The volume of initial data used is determined by the time factor, the budget for the work and the demands of the models available (Fig. 13). The information obtained at the initial stage
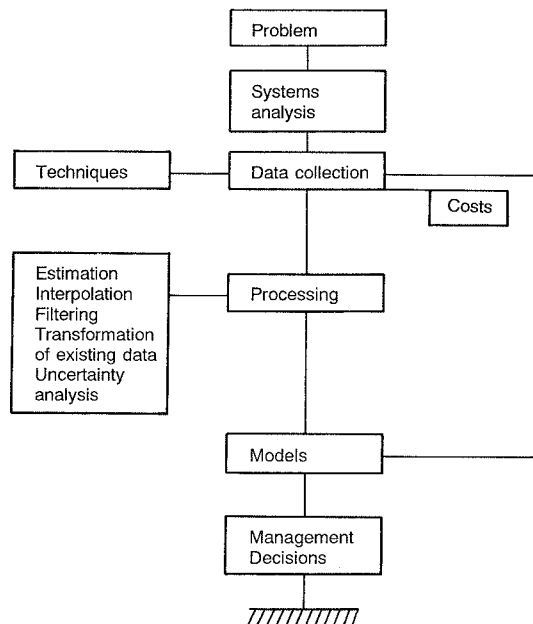

Fig. 13. Diagram showing the use of the data required for groundwater modelling (Fried and Bouman 1987).

should enable identification of the parameters required in modelling, the complexity and dimensions of the modelling, the geometry of the area, and the initial and boundary conditions. The data requirements to be considered for a predictive model are presented in Table 1. The accuracy of the modelling results is dependent on that of the input data, as indicated by the fact that each groundwater table observation contributes to the flow field to be modelled and a single erratic measurement may distort the hydrogeological interpretation of the whole area (van der Heijde et al. 1988).

3 THE AREA STUDIED

3.1 Quaternary deposits and groundwater geology

To the north of the village of Kärkölä the Younger Dryas end moraine complex Salpausselkä I runs from south-west to north-east (Fig. 14). The site studied here is located in a discontinuous esker chain of NW-SE orientation which lies in the foreland of the Salpausselkä zone, originating as a NE-SW ridge running beneath clay soils in the peatland area of Levijärvi (Figs. 14 and 15). The

Table 1. Generic list of input data for groundwater flow and solute transport modelling (after Mercer and Faust 1980a, Javandel et al. 1984, EPRI 1988, van der Heijde et al. 1988, Jensen 1988).

1 FLOW MODEL

Saturated zone	Unsaturated zone

– Data on geometry and geology of aquifer
  – boundaries of aquifer (physical and mathematical)
  – topography of bedrock and soil
  – location and character of geological structures (e.g., anticlines and synclines, faulting and river beds)
  – stratigraphy and spatial and temporal variation in thickness of soil layers
  – location of perched aquifer
  – hydraulic head, areal distribution and variations in hydraulic head
– Leakage from aquitard to aquifer
– Surface water features which act as recharge/discharge sites for the groundwater system
– Overflow of springs
– Water intakes: location and pumpage rate
  – Recharge areas (irrigation areas, recharge basins, recharge wells, etc.)
  – Recharge, evapotranspiration and precipitation
  – Areal distribution of hydraulic conductivity or transmissivity
  – Groundwater flow (rate and direction)
  – Areal distribution of storativity (confined aquifer) or specific yield (phreatic aquifer)
  – Porosity and effective porosity
	In addition to saturated zone:
	– Spatial and temporal variation in thickness of unsaturated zone
	– Geometry and continuity of soil layers, orientation of layers
	– Description of land surface relevant to infiltration and runoff
	– Distribution of porosity
	– Areal distribution and variation in capillary potential or moisture content
	– Dependences between different parameters
	  – capillary potential versus moisture content
	  – relative permeability versus capillary potential
	  – relative permeability versus moisture content

2 TRANSPORT MODEL

In addition to flow modelling:
- Solute dispersion data (e.g., diffusion/dispersion coefficient, longitudinal and transverse dispersivity
- Coefficients of reaction rate, equilibrium, etc.
- Areal distribution and variations in concentrations of the solute species in the system
- Information on present and future sources of contamination (e.g., rate of injection or leaching, chemical composition and concentration, position relative to aquifer)
- Background information on natural concentration distribution (water quality) in aquifer
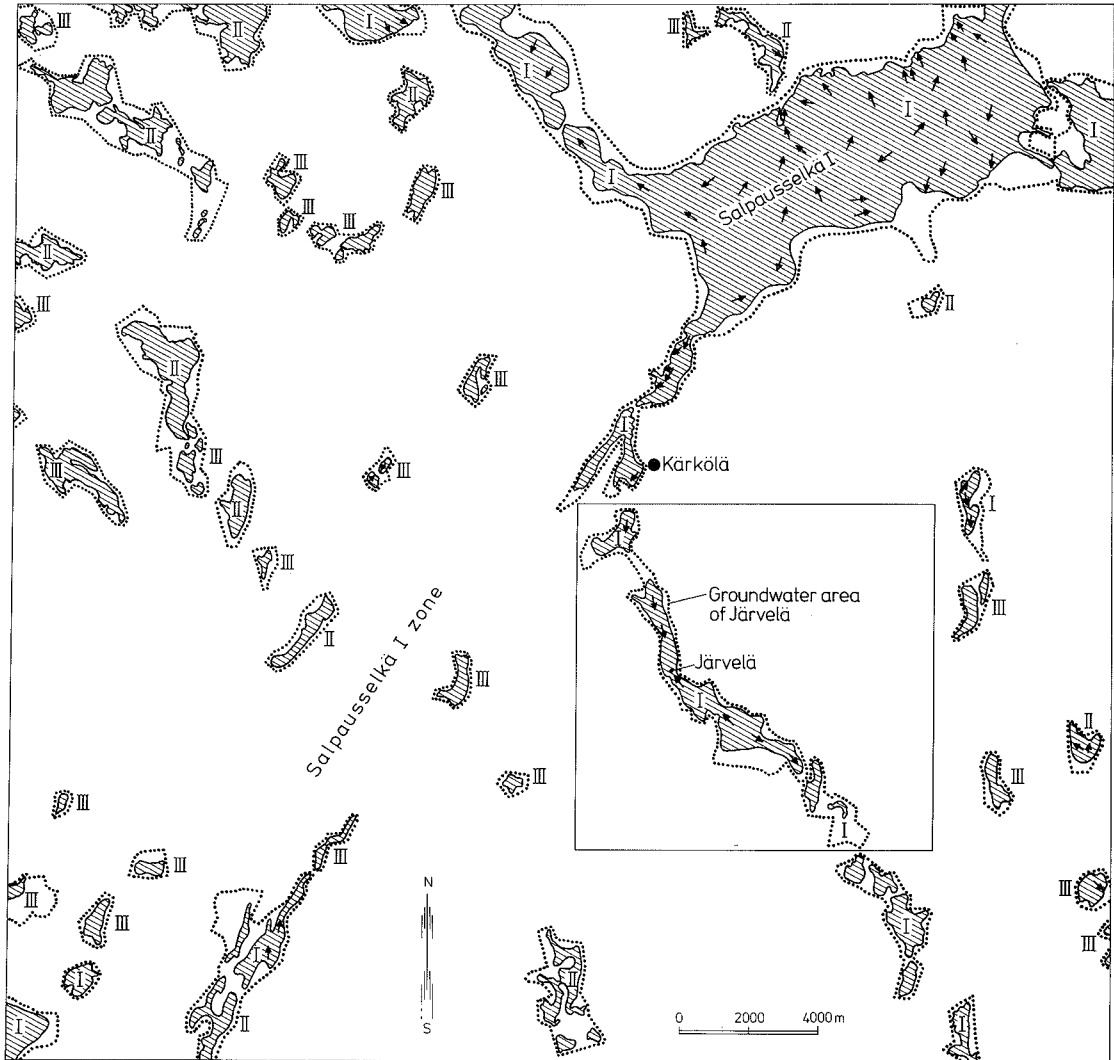
Legend:
— Boundary of groundwater recharge area
···· Boundary of groundwater area
➔ Main groundwater flow direction
Classification of aquifers:

I	= important groundwater supply area
II	= groundwater area suitable for water supply
III	= other groundwater area: evaluation demands further research

Fig. 14. Groundwater recharge areas – esker chains and Salpausselkä I – in general map sheet areas nos. 213304–213312, as defined by groundwater surveying and mapping (Britschgi et al. 1991, Helsingin vesi- ja ympäristöpiiri 1993a, 1993b, 1993c, 1993d, 1993e, 1993f, 1993g and 1993h). A more detailed map of the important groundwater area of Järvelä (no. 0431601) is presented in Fig. 15.
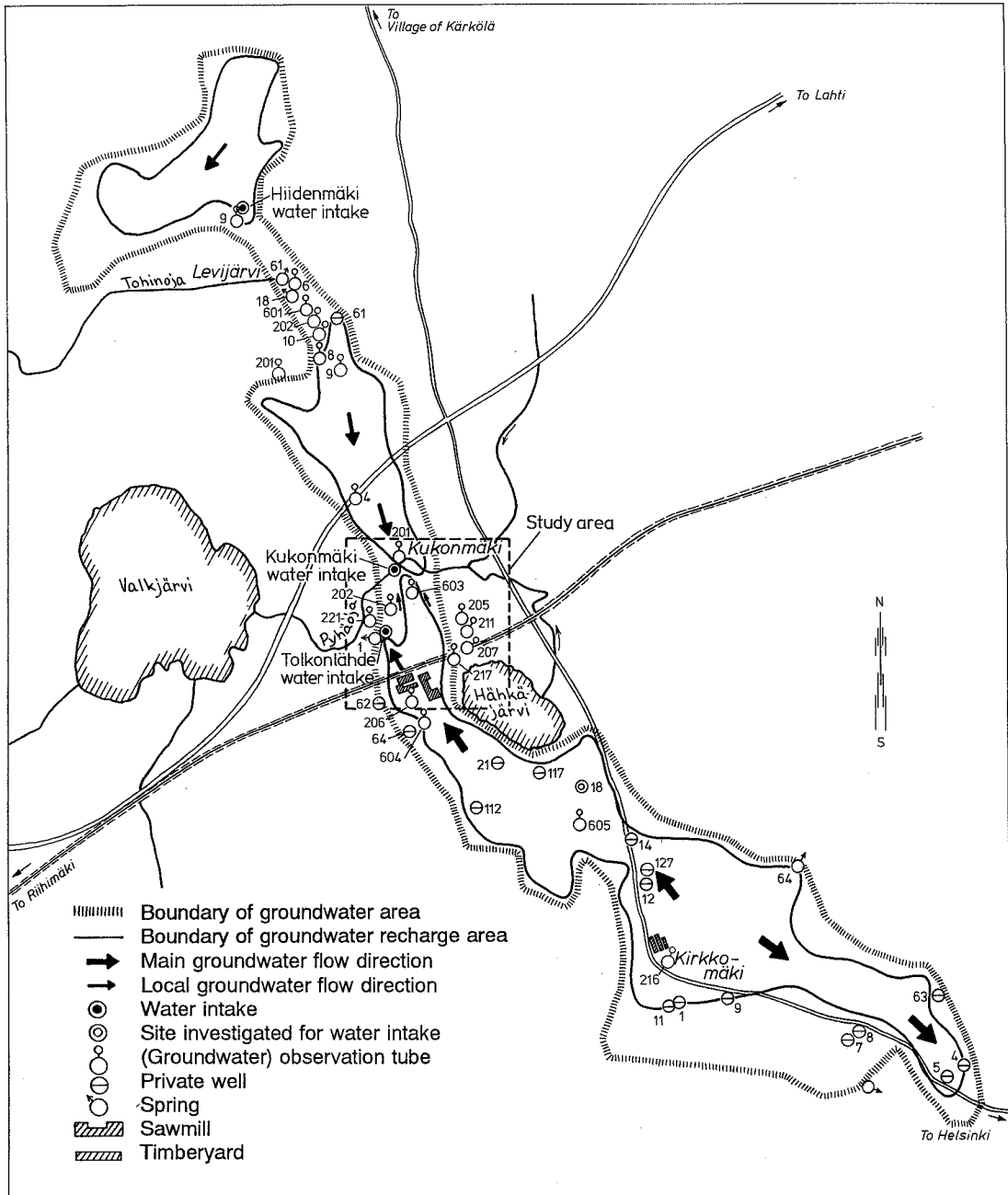
Fig. 15. The groundwater area of Järvelä (Helsingin vesi- ja ympäristöpiiri 1993e).
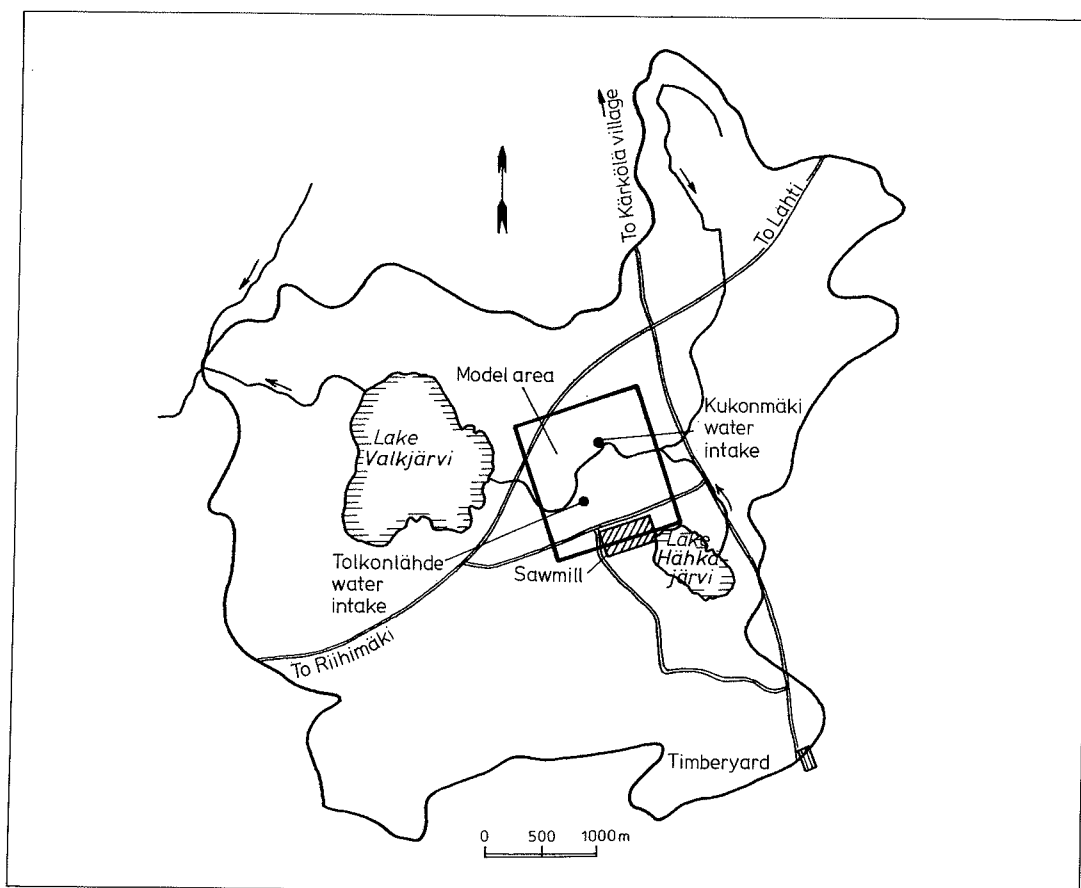
Fig. 16. The polluted part of the aquifer modelled here, located in the Valkoja drainage basin at Järvelä in the municipality of Kärkölä. The Valkoja drainage basin (no. 35.838) has an area of 24.1 km² (Granlund and Nystén 1991).

sequence continues towards the south-east in the form of the hill of Kukonmäki and as Kirkkomäki south of Pyhäoja. The direction of glacier movement varied between 315° and 330° around the esker chain in the area covered by general map sheets nos. 213307, 213308, 213310 and 213311 (Okko 1962, Grundström et al. 1991a, 1991b, 1991c, 1991d).

The area contaminated by chlorinated phenols forms part of the Järvelä groundwater area (no. 0431601 in Fig. 15), which is classified as an important groundwater area (class I) (Helsingin vesi- ja ympäristöpiiri 1993e). The Pyhäoja brook runs beside the Kukonmäki groundwater intake in the contaminated area and on to Lake Valk-järvi, situated in the Valkoja drainage basin approximately 1 km away from the area modelled (Fig. 16). The actual sawmill premises are located

south of the brook and the timberyard south-east of the brook and sawmill. The Kukonmäki water intake lies some 800 m away from the sawmill and approximately 3 400 m from the timberyard. There is another groundwater intake, Tolkon-lähde, 540 m north-west of the sawmill (Gran-lund and Nystén 1991, Nystén 1993).

The esker chain at Järvelä originated in a glacial meltwater tunnel or crevasse which later expanded and was finally filled with sand and gravel. The highest ridge of Kukonmäki, north of Pyhäoja, reaches $N_{60}+130$ m, while the summit of Kirkkomäki, some 3.5 km south of the brook, rises more than 30 m above its surroundings, to reach approximately 140 m a.s.l. (Fig. 15). The sea level at the margin of the retreating continental ice-sheet (Baltic Ice Lake I) was located some 150–156 m (Okko 1962, Donner

1969) above the present level on the line marked by the Salpausselkä I formation around 11 300–11 000 BP (Donner 1969, Repo and Tynni 1969, Niemelä 1971), which means that the entire area was covered by water and the glacial deposits were progressively subjected to the influence of littoral forces as they emerged.

This esker chain with a NW-SE orientation is covered by fine-grained sediments in places, the greatest thicknesses of which are recorded in the Pyhäoja depression marked by the brook Pyhäoja as it runs towards Lake Valkjärvi. The thickness of the clay beds at the point where the brook cuts through the esker chain has been shown to be 21 m (Insinööritoimisto Paavo Ristola Oy 1988a). Correspondingly, the fine-grained sediments on the lower reaches of Pyhäoja as it approaches Lake Valkjärvi have been shown to be 14 m thick and to have an average clay content of approximately 50 % (Grundström et al. 1991b). The clays around the Järvelä groundwater area are mostly underlain by till of low permeability. Highly permeable soils exist at the esker boundaries, at places extending beneath the clays which border on the eskers. The groundwater found in the fine-grained deposits occupied by the brook Pyhäoja constitutes artesian water.

The ground moraine surrounding the Järvelä groundwater area is composed of a sandy till with stones of normal size and a clay content of 2–3 %. Terminal moraines occur on the line of Salpausselkä I, comprising ridges of SW-NE orientation and composed, partially leached sandy till. The fines content of the ground moraine is usually so high and the material so dense that there is only enough groundwater to meet the demands of the individual households, although marked differences are observed in the permeability of the till both areally and between the strata. The till deposits observed are thin, as indicated by the frequent occurrences of bedrock terrain and the discontinuity of the strata (Grundström et al. 1991b, 1991c).

The esker chain in the Järvelä groundwater area consists primarily of highly permeable sands and gravels. The yield of the aquifer is 4 200 m^3 d^{-1}, as estimated from the recharge area and infiltration coefficient (Helsingin vesi- ja ympäristöpiiri 1993e). This rate is thought to be underestimated, and the estimated yield of the modelled area alone (Fig. 16) is set here at about 3 000 m^3 d^{-1}, as determined from the discharges

of the springs and the pumping rates. The coarsest-grained part of the area is located in the eastern section of the Kukonmäki ridge, which contains large kettle holes, and there are protruding clay wedges in the groundwater area which run towards the centre of the esker. The Kirkkomäki part of the esker contains thin layers of, wellsorted sands. There are also frequent occurrences of interfingering fine-grained layers in the esker (Helsingin vesi- ja ympäristöpiiri 1993e). Lake Hähkäjärvi, in the eastern part of the area, is a perched groundwater basin retained by clay beds.

In the part of the esker area north of Pyhäoja the groundwater is located at some depth, varying from +87 – +89 m to more than 40 m below the surface in the highest ridges of Kukonmäki. The groundwater is discharged from the esker chain through seepage flow and in the form of springs, and there is a natural discharge site at the Kukonmäki water intake north of Pyhäoja (Fig. 15), with an estimated yield of 720 m^3 d^{-1} (Helsingin vesi- ja ympäristöpiiri 1993e).

A water divide is located at Kirkkomäki, where the bedrock is overlain by 20–30 m layers of sand containing stones and boulders. In the southern part of Kirkkomäki the groundwater table lies at a depth of approximately 7 m (Grundström et al. 1991c), while in the delta section of the ridge, at a soil extraction pit south of Lake Hähkäjärvi, it lies at only 3 m, i.e. at a level of +96 m. The primary direction of groundwater flow in the area north of Kirkkomäki is north-westwards, away from the hill, to discharge mainly at Tolkonlähde, which has an estimated average yield of 1 300 m^3 d^{-1} (Helsingin vesi- ja ympäristöpiiri 1988). A groundwater intake has been constructed at this spring south of Pyhäoja (Fig. 15).

3.2 Bedrock geology

The metamorphosis which took place in the area covered by the Kärkölä map sheet (no. 2133) has generally destroyed almost all the structural features typical of supracrustal rocks (Fig. 17). There is occasional banding, which points to original stratification, with dispersed grains of uralite and plagioclase phenocrysts, suggestive of volcanic origin. The schistosity corresponds in direction to the original stratification, and the
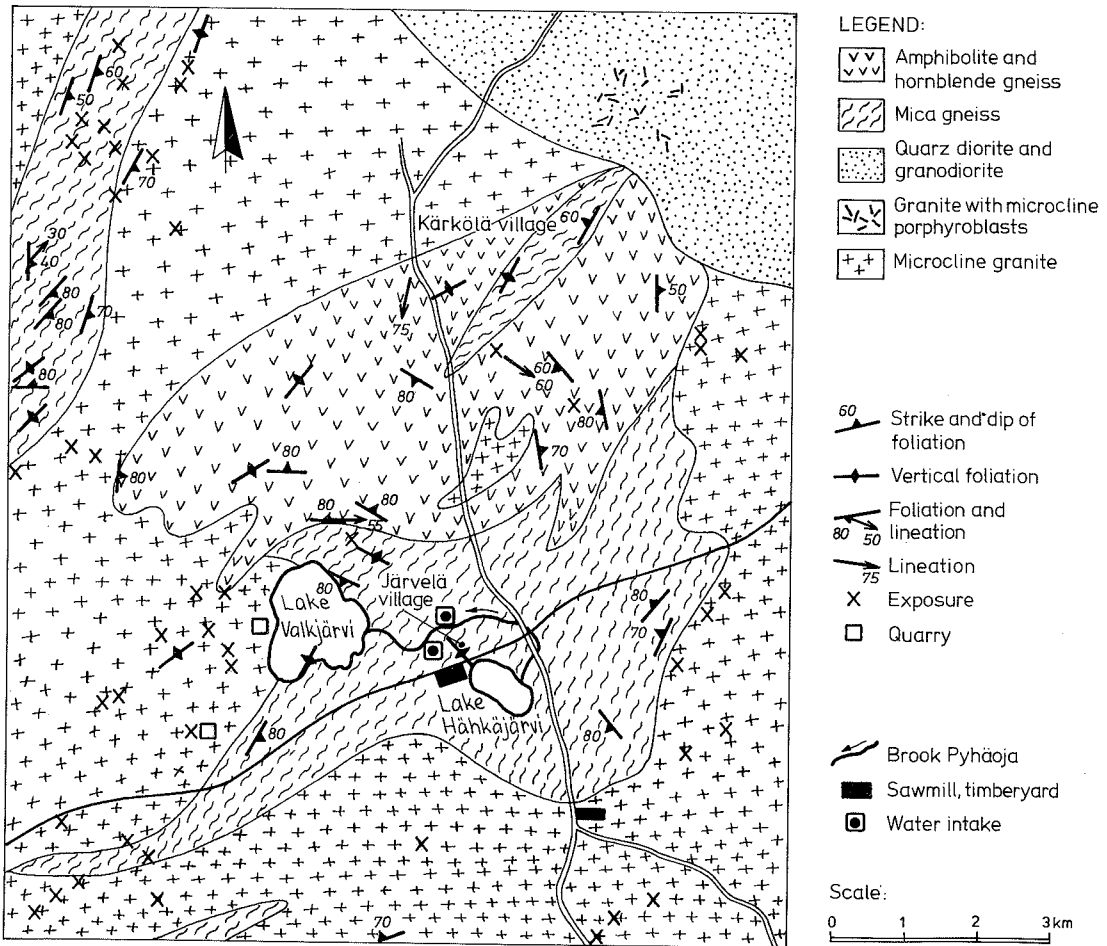
Fig. 17. Pre-Quaternary rocks of the Kärkölä area (simplified after Lehijärvi, 1961).

weathering products have been altered to mica gneisses and coarse-grained garnet-cordierite gneisses. Basic vulcanic rocks occur in the form of hornblende gneisses, and the mica gneisses are markedly veined. The mica gneisses often have alternating layers of amphibolite and hornblende gneiss associated with them (Lehijärvi 1962).

The polluted groundwater area lies in a mica gneiss area within a granite massif, while there is vertically dipping schistosity in the bedrock in the area between the sawmill and the Kukonmäki groundwater intake (Fig. 17). The veined gneiss around Järvelä is partly garnet-bearing and partly cordieritic. The area south of the village of Kärkölä is primarily composed of coarse-grained hornblende gneiss and biotite-hornblende gneiss (Lehijärvi 1962).

The area covered by the Kärkölä map sheet forms part of a zone dominated by microcline granite which extends from the coast of southwestern Finland to the Viipuri rapakivi region. The proportion of quartz-dioritic rocks is markedly smaller, while no rocks of a more basic composition are recorded on the map (Lehijärvi 1962).

The microcline granite which is the principal

rock in the Kärkölä area is usually red, but may be greyish or very light in colour. Its grain-size distribution varies from coarse to medium, and it tends to be inhomogeneous, largely on account of these fluctuations in grain-size and the presence of both faint traces and well-preserved remains of older rock types. It is also very common for the microcline grains and biotite scales to occur in parallel, occasionally yielding the rocks a distinctive orientation which corresponds to that of the schistose remnants. The schists are vertical or steeply inclined in dip (Lehijärvi 1962).

Most of the north-eastern part of the map area (Fig. 17) is designated as quartz granodiorite, but this is largely hypothetical, on account of the lack of outcrops. Observations at outcrops in the middle of the defined quartz granodiorite area indicate the presence of microcline-porphyroblastic granite (Lehijärvi 1962).

Lehijärvi (1962) suggests fracture lines for the Kärkölä map sheet which occur in the form of valley chains, river beds and longitudinal orientations of lakes. The distribution of bedrock outcrops is uneven. There are only a small number of outcrops in the polluted groundwater area studied here, and these together with aeromagnetic maps (Geologian tutkimuskeskus 1988, Geological Survey of Finland 1988) fail to indicate any fracture zones in the Järvelä area.

In general, the surface of the bedrock in the area of the Kärkölä map sheet is irregular and the relative differences in height are fairly large in places, although no parts of the bedrock in the area studied here rise as high as the highest parts of the Järvelä esker chain. According to Okko (1962), the topography of the bedrock is of preglacial origin, and the bedrock surface provided both channels for glacier flow and obstructions to it. The morphological depressions were eroded by continental ice. The valleys in which the rivers run are sometimes bordered by outcropping bedrock with almost vertical slopes. The morphological depressions in the bedrock are filled with till, glacial sediments and peat. Thus the bed of the Pyhäoja brook, for example, located beside the Kukonmäki water intake lies, on the fine-grained deposits beneath which are permeable sediments. Without detailed investigations, it is difficult to estimate the degree to which fracturing is reflected in the topography (see Niini 1968, Niini et al. 1972, Rönkkö 1968).

4 RESEARCH METHODS

4.1 Field investigations

4.1.1 Soil and groundwater sampling

Investigations were performed in 1986–1987 as part of the obligatory supervision measures ordered by the Helsinki Water and Environment District in order to examine the chlorinated phenol content of the soil and groundwater around the sawmill and its timberyard (Insinööri-ja limnologitoimisto Oy Vesitekniikka Ab, 1986a, 1986b, Insinööritoimisto Paavo Ristola Oy 1987). In autumn 1987 concentrations of 4.1 µg l^{-1} were recorded in the brook Pyhäoja near the Tolkonlähde water intake (Fig. 16). Further measures were then taken immediately upon the discovery of groundwater pollution at the Kukonmäki water intake in December 1987 in order to define the extent of the occurrence of the chlorinated phenols (Fig. 18). The chlorinated phenol content of the water at the intake exceeded the limit of 10 µg l^{-1} recommended by the National Board of Medicine approximately by a factor of ten, which led to its closure, while concentrations of approximately 800 µg l^{-1} were recorded in the brook Pyhäoja (Nystén 1988, 1989, 1990, 1991a, 1991b, 1993). The necessary investigations were launched by the Helsinki Water and Environment District in spring 1988 (Herkamaa 1988). The latest investigations into the soil of the sawmill area were completed in autumn 1990 for the purposes of the ensuing legal proceedings (Geosto Oy 1990) and in 1991 for hearings at the Supreme Administrative Court (Geosto Oy 1991). The groundwater head and chlorinated phenol concentrations in the Järvelä area are monitored continuously twice a year. In addition, further fieldwork was launched for restoration of the polluted aquifer by Helsinki Water and Environment District in 1993.

The use of the compound Ky5 and other toxic substances in this groundwater area was assessed, and preliminary data obtained on the stratigraphy of Quaternary deposits, location of the bedrock surface and earlier excavation work in the area by examining the history of construction work carried out at the sawmill, in its timberyard and in the surrounding area. Well site investigations were performed in the area between the sawmill and the groundwater intakes, and water samples

were obtained from private wells, the water intakes and the brook Pyhäoja. Information was also available on investigations for the identification of a suitable groundwater intake commissioned by the local authorities (Insinööritoimisto Paavo Ristola Oy 1973) and groundwater surveys commissioned by the timber company in the area between the sawmill and the Kukonmäki water intake (Insinööri- ja lim-nologitoimisto Oy Vesitekniikka Ab 1986a, 1986b; Insinööritoimisto Paavo Ristola Oy 1987, 1988a, 1988b). Other research commissioned in the area included soil-rock penetration tests, installation of groundwater observation tubes and
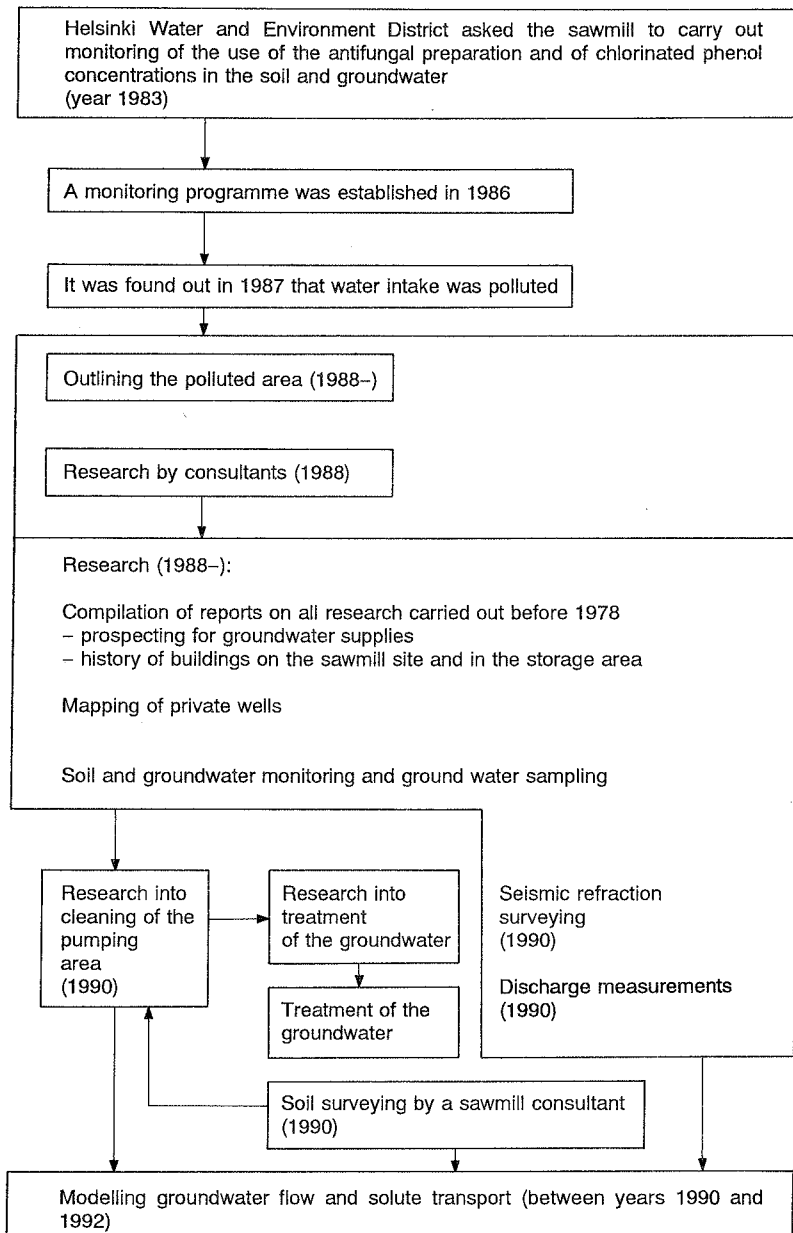
Fig. 18. History of research into the polluted aquifer. All the surveillance data were available for this modelling study.

soil and groundwater sampling.

The 22 groundwater tubes were installed using heavy drilling equipment (Oy Vesi-Hydro Ab 1988a, 1988b), as the area features compacted strata which were occasionally over 30 m thick and the aim was to extend drilling to the underlying bedrock. At some sites the drill was allowed to penetrate the bedrock in order to examine its degree of fracturing and the amount of groundwater contained in the bedrock. The sediment types were identified in the field and the presence of chlorinated phenol content in the soil samples assessed preliminarily on the basis of smell. Some of the samples were sent to the laboratory for grain-size and permeability determinations and chemical analyses. Compressed air was used to clean the boreholes wherever possible. Soil samples for chlorinated phenol content analysis were also collected from

the sawmill area by means of an excavator and multi-purpose and weight-operated corers (Fig. 19).

Plastic groundwater tubes of diameter 50 mm or 63 mm and one iron groundwater tube of diameter 32 mm were installed in the boreholes and extended as far as the bedrock (Fig. 20). The screen parts of these tubes passed through the entire saturated zone. Water samples were obtained primarily through pumping, and from three tubes by means of a sampler.

The hydraulic head of groundwater was measured by means of a probe before pumping, and has been monitored ever since spring 1988. The heads tend to vary according to season and changes in groundwater pumping conditions. The values obtained were used to check for any clogging of the tubes and to monitor perched groundwater levels.

Fig. 19. Locations of soil samples for chemical analysis taken by excavator and by drilling at the sawmill in 1988. The numbered irrigation basins (from 1 to 4) and their years indicate the places where the basins have been situated at different times. There was fire at the sawmill in 1976, and the old buildings (between 1957 and 1976) are marked with dense shading and the new buildings (between 1976 and 1993) with sparse shading.

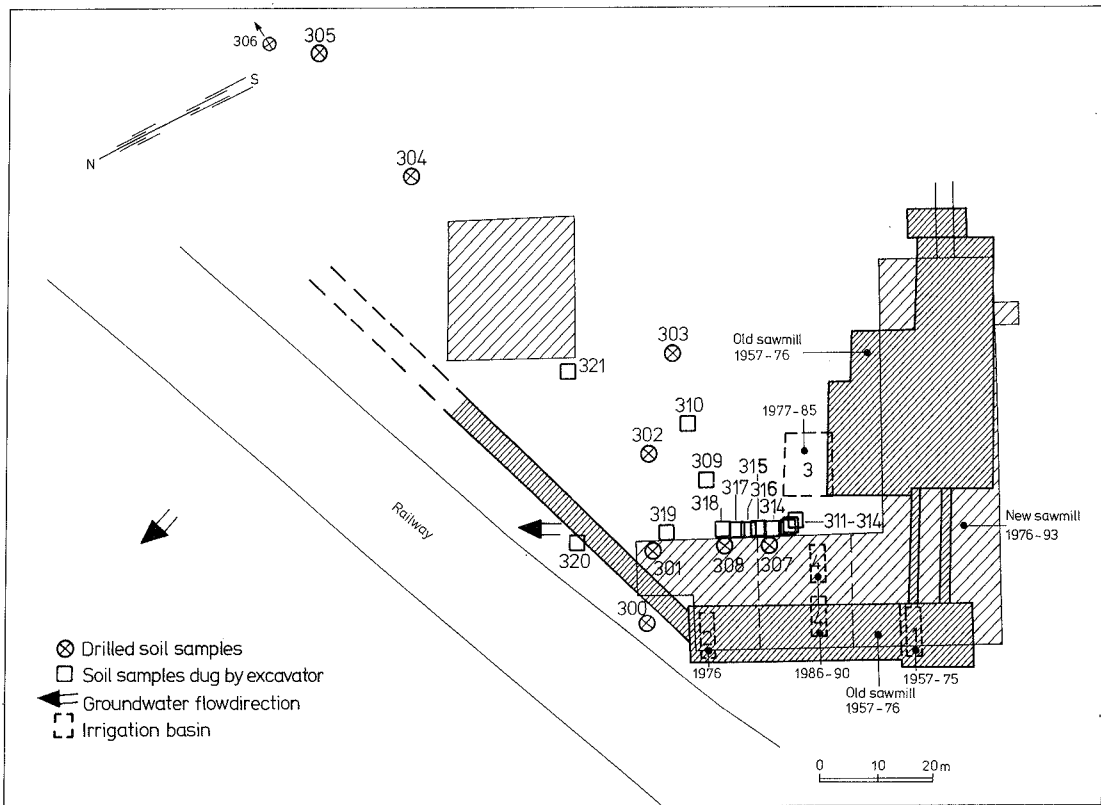Water and soil samples were analysed for the tri-, tetra- and pentachlorophenols contained in Ky5, and some of the samples were analysed for their disintegration and alteration products. Attention was also paid to the Kemtox S10 currently used by the company. The occurrence and concentrations of chlorinated phenols in the groundwater are now being monitored regularly in spring and autumn.

4.1.2 Seismic soundings

The aim of seismic refraction surveys was to identify the types of Quaternary deposits, the location of the bedrock surface, the positions of bedrock ridges which could interfere with groundwater flow, and the quality of the bedrock. Geophones were installed at intervals of five metres on the sounding lines and blasting points at 25 m intervals (Terraplan Oy 1990). An ABEM Terraloc Mk III seismograph was used for recording purposes. The sounding lines, with a total length of 1 650 m, are shown in Fig. 21.

The idea of the seismic refraction method is that the velocity of the seismic waves reflects the characteristics of the geological stratum concerned (Fig. 22). The method usually enables depth to be determined with a deviation of less than one metre when the thickness of soil cover is less than 10 m or to an inaccuracy of less 10 % in the case of greater thicknesses (Taanila 1965).

The effect of rock quality on the seismic velocity is estimated by Öhberg and Ihalainen (1988) to vary according to the degree of fracturing, and it is also known to be affected by the rock type (Fig. 23). The inaccuracy of such determinations is usually ±200 m s⁻¹ (Peltoniemi 1988).

4.1.3 Discharge measurements

Measured groundwater yield values for the period 1970–1991 are available to serve as estimates of the rates of groundwater flux via the boundaries of the area modelled. Groundwater research was performed in the Järvelä groundwater area in the 1970's for water supply purposes, and research including pumping tests and measurements of the overflow of artesian springs and seepage and stream flow in the brook Pyhäoja was carried out
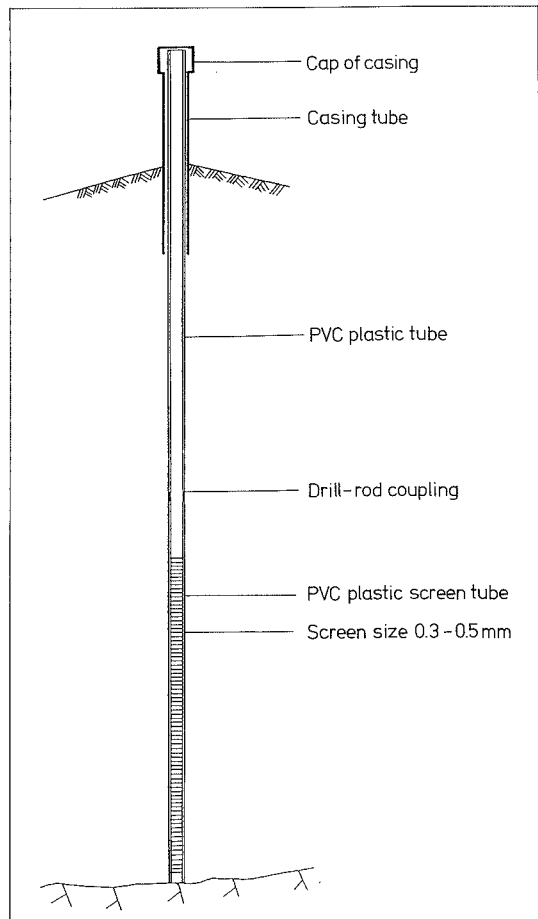
Fig. 20. An observation tube used for water sampling and hydraulic head measurements (Herkamaa 1988).

in order to select a suitable site for a water intake (Insinööritoimisto Paavo Ristola Oy 1973). Discharge measurements were also performed during the spring and autumn runoff periods in 1990 (Fig. 21). In addition, water supply monitoring data were available for the water intakes at Tolkonlähde and Kukonmäki both before and after contamination.

4.2 Laboratory tests

The sediment samples were examined for grain-size distribution and permeability at the soils laboratory of the Water and Environment Research Institute. Grain-size distribution was
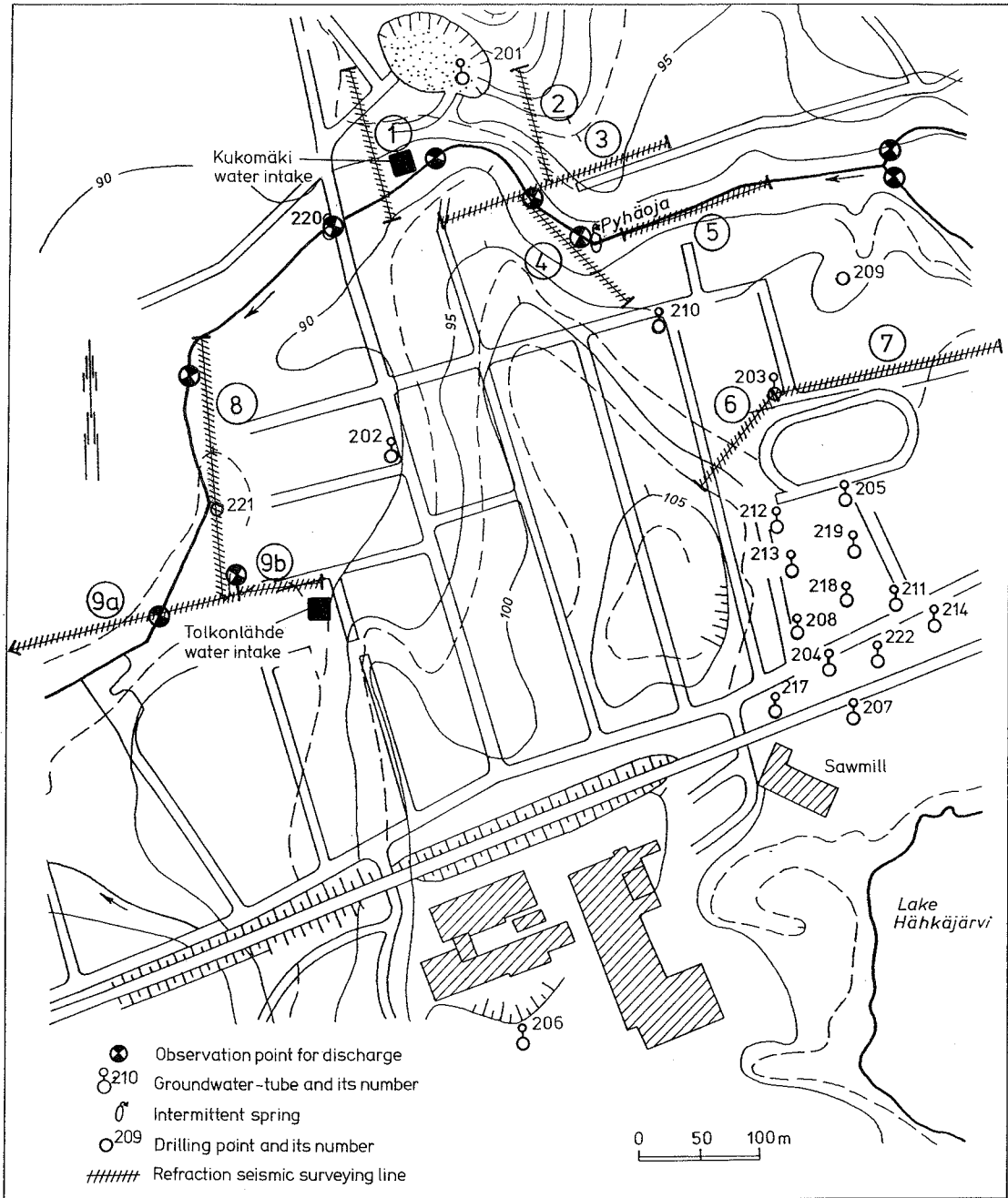
Fig. 21. Location of groundwater tubes, surveying lines (1–9) for seismic refraction soundings and observation points for discharge (calculated using a programme developed by the Hydrological Office of the Water and Environment Research Institute; Sucksdorff and Kleemola 1986).

determined from 14 samples by means of a sedigraph. Three examples of grain-size distribution curves are presented in Fig. 24. In addition, 11 sediment samples were subjected to constant head permeability tests.
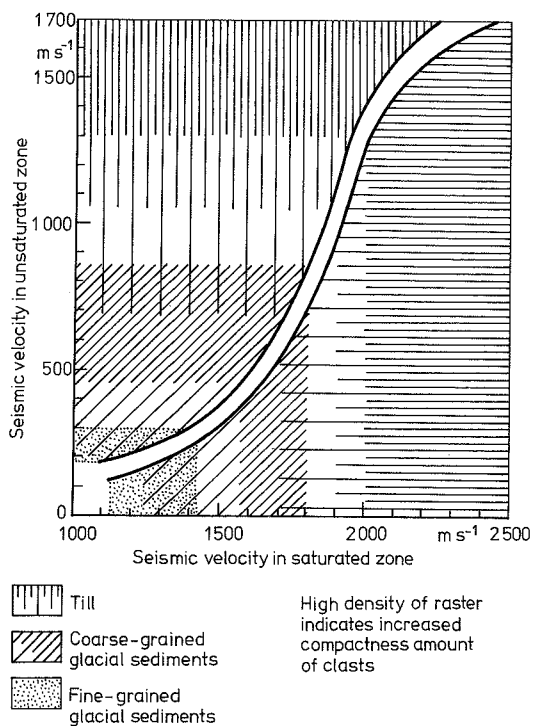
A total of 35 sediment samples were analysed for chlorinated phenols at the Chemical Laboratory of the Technical Research Centre of Finland and 19 at the same organization's Food Research Laboratory. The samples were first air-dried and then passed through a sieve with a 2 mm mesh. The samples dug by excavator were examined by gas chromatography/mass-spectrometry employing the selected ion monitoring (SIM) technique. The chlorinated phenol concentrations of the core samples were determined in terms of acetyl ester derivatives identified in their acid ether extracts, using 2,4,6-tribromophenol as an internal standard. The samples were analysed by gas chromatography using an EC detector and their chlorinated phenol concentrations calculated in microgrammes per kilogramme of sample (dry weight). The detection limit was 2 µg kg^{-1}.

In addition to chlorinated phenols, the 17 soil samples were also examined for the Kemtox S10 preservative at the Chemical Laboratory of the Technical Research Centre of Finland. The harmful substances contained in this agent are 2-(thiocyanomethylthio)benzothiazole (TCMTB 12 %) and 2-n-octyl-4-isothiazolin-3-one (OIT 4.5 %). The soil samples were extracted with a mixture of methanol-acetonitrile azeotrope. The analysis was performed by liquid chromatography and quantification was based on the external standard. Concentrations were expressed in mg per kilogramme of sample (dry weight), with detection limits of 0.2 mg kg^{-1} for TCMTB and 0.5 mg kg^{-1} for OIT. The analytical method is based on the description of the liquid

Fig. 22. Seismic velocities of soil types lying above and below the groundwater table. Soil layer velocities increase if the soil is tighter and the grain size coarser (RIL 1976, modified from Taanila 1965).

Fig. 23. Seismic velocities of given rock qualities (after Öhberg and Ihalainen 1988, who modified the rock quality classification from Barton et al. 1974). Rock type is disregarded.

chromatographic analysis of preservative-treated timber given by Kennedy (1986, p. 701–705).

The groundwater samples obtained at the early stages of the research carried out by Helsinki Water and Environment District were analysed in external laboratories on account of the insufficient capacity of the own laboratory in relation to the large number of samples involved. Thus the comparative measurements of chlorinated phenols performed in autumn 1988 (Table 2) involved the participation of Insinööritoimisto Paavo Ristola Oy (Engineers), DN-Bioprocessing Oy, the Food Research Laboratory of the Technical Research Centre of Finland or the Research Laboratory of the Water and Environment Research Institute. In order to ensure comparability of the results, however, subsequent measurements in spring and autumn of each year have primarily been performed in the Research Laboratory of the Water and
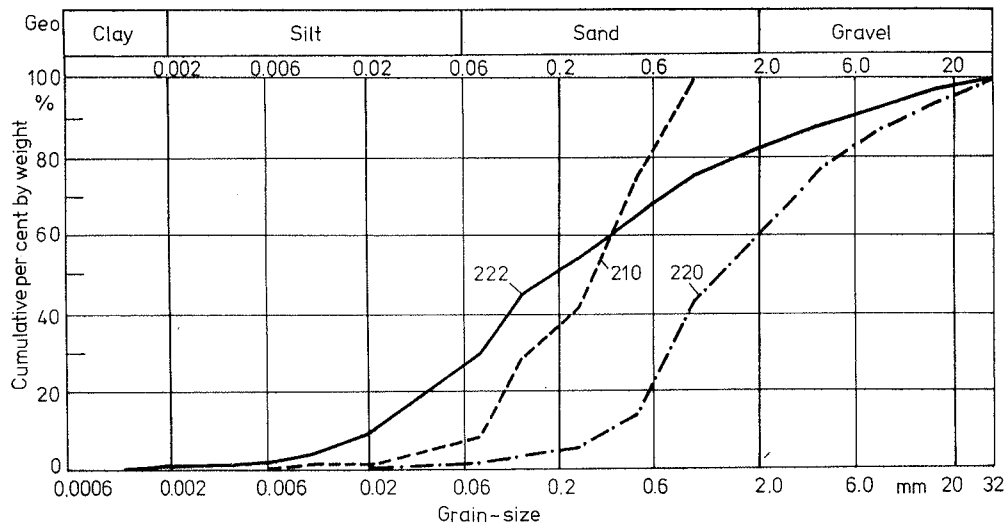
Fig. 24. Grain-size distribution of samples 210, 220 and 222.

Table 2. Results of the comparison of chlorinated phenol determinations.

Sample	Analysis		Laboratory 1	Laboratory 2	Laboratory 3	Laboratory 4
Sample A	TCP	$\mu g\ l^{-1}$	<0.01	3.0	4.1	11
	TeCP	$\mu g\ l^{-1}$	3.0	32*/27**	18	2.0
	PCP	$\mu g\ l^{-1}$	0.6	1.3*/1.4**	1.2	1.0
Sample B	TCP	$\mu g\ l^{-1}$	7.0	1.7	..	..
	TeCP	$\mu g\ l^{-1}$	15	7.9*/7.5**	..	..
	PCP	$\mu g\ l^{-1}$	0.7	0.38*/0.42**	..	..
Sample E	TCP	$\mu g\ l^{-1}$	23	4.8	250	..
	TeCP	$\mu g\ l^{-1}$	590	460*/420**	280	360
	PCP	$\mu g\ l^{-1}$	26	25*/25**	267 000$	..

*/**	= asetylated/methylated
$	= probable analysis mistake
..	= not analysed
PCP	= pentachlorophenol
TCP	= trichlorophenol
TeCP	= tetrachlorophenol

Environment Research Institute. In addition to these, supervision samples have been taken by the sawmill operators and analysed in the Control and Investigation Laboratory of Lahti since 1989.

The Research Laboratory of the Water and Environment Research Institute used both the methylation and the acetylation method in the analyses. In the former case an acidified water sample was extracted with chloroform $(40+30+30$ ml $l^{-1})$, concentrated and methyl-derivatized with diazomethane, after which an internal standard was added (2,4,6-tribromophenol and/or 2,3,6-trichlorophenol) and the analysis of a hexane solution was performed by gas chromatography/ECD. In the acetylation method, 2,3,6-trichlorophenol as an internal standard, potassium carbonate buffer and acetic anhydride were added after adjustment of the pH and the resulting acetyl derivatives were extracted in hexane and analysed by gas chromatography/ECD. Quantification was based on the internal standard.

4.3 Groundwater modelling

4.3.1 Finite difference grid and data requirements for the present model

The area to be modelled here was approximately 1 km^2 in size and the grid was designed on geological grounds. Its impermeable boundaries are composed of rock and clay soils. The grid covered the entire area, being of size 24 x 26 squares, with a node interval of 42.7 m (Fig. 25). Areal variation of the parameters and variable boundary . conditions were taken into consideration when creating the grid. Of the parameters included in the model, the soil permeability properties, i.e. hydraulic conductivity (K) and transmissivity (T), were determined, whereas groundwater flow was assumed to be steady. Conditions at the boundaries were determined from the hydraulic heads.

The following initial data were examined in the course of the modelling:

(1) Aquifer geometry and structure
– aquifer boundaries
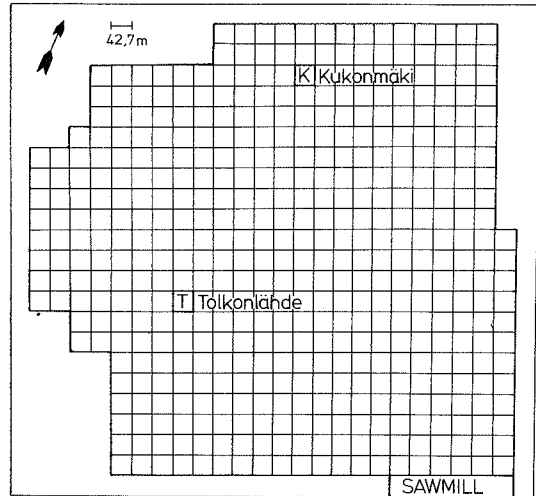
Fig. 25. Grid used for studying the aquifer.

– location of bedrock surface
– hydraulic head and its variations
– stratigraphy
– hydraulic conductivity (determined by the constant head permeability test and indirectly on the basis of grain-size distribution and soil types)

(2) Factors affecting groundwater storage
– relation between surface water and the aquifer
– perched groundwater
– overflow of artesian and seepage springs and stream flow in the brook
– number and location of water intakes and pumping rate
– precipitation
– infiltration coefficients
– rate of flux via the boundaries

The source data used in the final calibrated model will be presented below in section 5.3.

4.3.2 MOC groundwater model equations and main assumptions

The computer model MOC (Method of Characteristics; modified version IBM-PC 2.5) is a two-dimensional finite difference transport model. The program solves two simultaneous partial differential equations: a groundwater flow

equation which describes the distribution of the hydraulic head in the aquifer, and a solute transport equation which describes chemical concentrations in the system. By coupling the two, the model can be applied to both steady-state and transient flow problems. Either groundwater heads or flow rates can be used as boundary conditions, and the initial condition can be the hydraulic head or the pollutant concentration, for example. The model assumes that no reactions occur that affect the concentration of the substance of interest, and that the fluid density, viscosity and temperature gradients do not affect the velocity distribution. However the aquifer may be heterogeneous or anisotropic (Konikow and Bredehoeft 1984).

Flow equation

The equation describing the transient two-dimensional areal flow of a homogeneous compressible fluid through a nonhomogeneous anisotropic aquifer can be written as (7)

$$\frac{\delta}{\delta x_i}\left(T_{ij}\frac{\delta h}{\delta x_j}\right) = S\frac{\delta h}{\delta t} + W \qquad i, j = 1, 2 \qquad (7)$$

where

T_{ij}	is the transmissivity tensor;
h	is the hydraulic head;
S	is the storage coefficient;
t	is the time;
$W = W(x,y,t)$	is the volume flux per unit area (positive sign for outflow and negative for in flow); and
x_i and x_j	are the Cartesian coordinates (Konikow and Bredehoeft 1984).

If the only fluxes considered in (7) are direct withdrawal or recharge, i.e. well pumping, well injection, or evapotranspiration, and those in (8) are steady leakage into or out of the aquifer through a confining layer, stream bed or lake bed, then $W(x,y,t)$ may be expressed as

$$W(x, y, t) = Q(x, y, t) - \frac{K_a}{m}(H_s - h) \qquad (8)$$

where

Q	is the rate of withdrawal (positive sign) or recharge (negative sign);

K_a	is the vertical hydraulic conductivity of the confining layer, streambed, or lakebed;
m	is the thickness of the confining layer, streambed, or lakebed; and
H_s	is the hydraulic head in the source bed, stream, or lake (Konikow and Bredehoeft 1984).

An expression for the average seepage velocity, of ground water can be derived from Darcy's law. This expression can be written as

$$V_i = -\frac{K_{ij}}{\in}\frac{\delta h}{\delta x_j} \qquad (9)$$

where

V_i	is the seepage velocity in the direction of x_i;
K_{ij}	is the hydraulic conductivity tensor; and
$\in$	is the effective porosity of the aquifer (Konikow and Bredehoeft 1984).

Transport equation

The equation used to describe the two-dimensional areal transport and dispersion of a given non-reactive dissolved chemical compound in flowing groundwater may be written as

$$\frac{\delta(Cb)}{\delta t} = \frac{\delta}{\delta x_i}\left(bD_{ij}\frac{\delta C}{\delta x_j}\right) - \frac{\delta}{\delta x_i}(bCV_i) - \frac{C'W}{\in}$$

$$i, j = 1, 2 \qquad (10)$$

where

C	is the concentration of the dissolved chemical compound;
D_{ij}	is the coefficient of hydrodynamic dispersion (a second-order tensor);
b	is the saturated thickness of the aquifer; and
C'	is the concentration of the dissolved chemical in a source or sink fluid.

The first term on the right-hand side of equation 10 represents the change in concentration due to hydrodynamic dispersion, the second term describes the effects of convective transport, and

the third term represents a fluid source or sink (Konikow and Bredehoeft 1984).

A number of assumptions were made when developing the above equations, including the following major considerations that must be carefully evaluated before applying the model to the solution of a field problem (Konikow and Bredehoeft 1984).

1. Darcy's law is valid, and hydraulic head gradients are the only significant driving mechanism for fluid flow.
2. The porosity and hydraulic conductivity of the aquifer are constant with time, and the porosity is uniform in space.
3. The fluid density, viscosity and temperature gradients do not affect the velocity distribution.
4. No chemical reactions occur that affect the concentration of the dissolved chemical, the fluid properties or the properties of the aquifer.
5. Ionic and molecular diffusion are negligible contributors to the total dispersive flux.
6. The vertical variations in head and concentration are negligible.
7. The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

The program uses an alternating direction implicit (ADI) procedure to solve a finite difference approximation to the groundwater flow equation and the method of characteristics to solve the transport equation. The latter represents convective transport by means of a particle tracking procedure and solves the finite difference equation that describes the effects of hydro-dynamic dispersion, fluid sources and sinks and the velocity divergence by means of a two-step explicit procedure. For each time step, every particle is moved a distance proportional to the length of the time increment and the velocity at the location of the point (Konikow and Bredehoeft 1984).

The program, written in FORTRAN IV, contains about 2 000 lines and is segmented into a main routine and eight subroutines. The general program is written to deal with a difference grid having up to 20 rows and 20 columns. The grid of MOC model used at the Water and Environment Research Institute has been enlarged to represent 30 columns and 40 rows. Thanks to the good documentation, changes can be made to the code in the course of the work. This modified version of the MOC model is not very easy to use, due to the slowness and complexity of feeding in the data.

5 RESULTS

5.1 Regional geology

The seismic sounding results are averages for the sounding points and their immediate surroundings, as a consequence of which rock surface and soil type data were compared with drilling results for interpretation purposes. The lines employed in the seismic refraction soundings are depicted in Fig. 26 and examples of the geological stratigraphy in Figs. 27, 28 and 29. It was impossible to determine the velocity in the rock on lines 1–4 due to the shortness of the lines and thickness of the surficial deposits.

Information on bedrock depth and quality was obtained by extending the drilling to the rock surface and by means of excavations and seismic refraction soundings (Figs. 19 and 21). No fracturing was observed in the bedrock in the main pars of the modelled area, the bedrock depression or the Pyhäoja valley (Figs. 26, 27, 29, 30 and 31), but some was to be found in the Pyhäoja area north-west of Tolkonlähde (Fig. 28). The effect of rock type was not taken into consideration when interpreting the bedrock quality, as the seismic velocities indicated on the cross-sectional drawings are mean values calculated by a sampling method. In any case, rock type affects seismic velocity less than does fracturing, particularly at velocities of less than 4 500 m s^{-1}.

Investigations performed between the sawmill and the Kukonmäki groundwater intake indicated that the area can be divided into parts representing the esker, a bedrock ridge, the bedrock depression and the valley (Fig. 32). The soil of the esker area is composed of highly permeable sand and gravel layers of thickness from 15 to 30 m covered by clay and silt at low-lying points. The water intakes of Tolkonlähde

Fig. 26. Seismic refraction surveying lines 1–9 and their velocities in the bedrock where it was possible to determine them. The velocities are between 3 500 and 4 000 m s^{-1} in fractured bedrock and over 4 500 m s^{-1} in massive or sparsely jointed bedrock. No velocities in the range 4 000–4 500 m s^{-1} (abundantly jointed) or under 3 500 m s^{-1} (crushed rock) have been recorded in this area. For key to missing symbols, see Fig. 21. Cross-sections of surveying lines (6–7), (207–201) and (9b–8) are shown in Figs. 27, 28 and 29.

and Kukonmäki are located on this esker chain (Herkamaa 1988, p. 604–605).

The sediments deposits of the bedrock depression area are mainly composed of fine-grained, poorly permeable deposits which grade to sand and till deposits with depth (Figs. 27 and 29). The sediments deposits in the depression are from 0.5 to 20 m in thickness, but decrease to less than 0.5 m near the Ky5 impregnation sites at the sawmill (Figs. 30 and 31). The bedrock surface slopes towards the Kukonmäki water intake in the Pyhäoja valley (Fig. 27). The eastern boundary of the bedrock depression was identified at sounding line no. 7 and at observation tube no. 214 north-east of the sawmill. In addition, the deposits become poorly permeable east and north of the sports ground.

The north-south-oriented bedrock ridge acts as a local groundwater divide between the esker area and the bedrock depression. It terminates at the Pyhäoja valley, which contains sand and gravel of

thickness approximately 20 m overlain by fine-grained material (Fig. 32).

The groundwater head is located at average depths of 4–10 m between the sawmill and the contaminated water intake, with groundwater discharging into Pyhäoja. The total thickness of the saturated zone exceeds 30 m in places. The bedrock depression of the Pyhäoja valley continues northwards beneath the esker chain. The average level of the bedrock around the Kukonmäki water intake and in the valley itself is +60 m (Fig. 27), as indicated by the drillings and the seismic survey lines 1–5. The soundings indicate that the deepest points in the bedrock surface correspond to the location of Pyhäoja (lines 1–5 and 8–9, Fig. 26).

At the time of the contamination of the Kukonmäki water intake, the direction of groundwater flow in the esker area was from the south and north, primarily towards the water intake, and also from the south towards
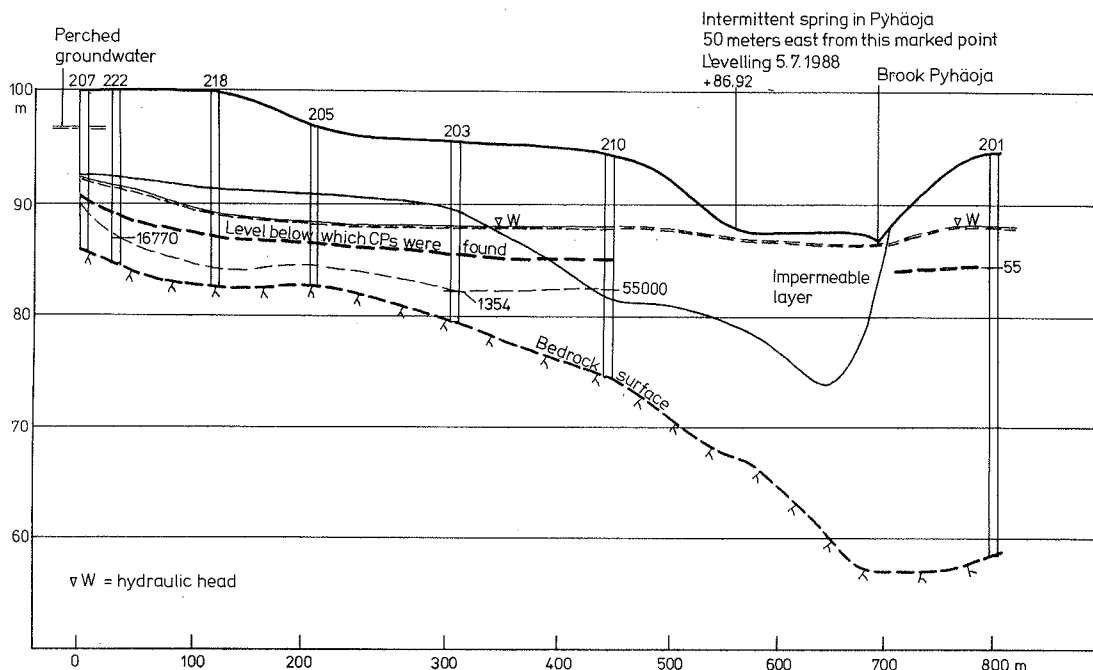
Fig. 27. Cross-section along the same surveying line (207–201) as in Fig. 26 between the sawmill and the water intake area. The groundwater head is near the bottom of the brook Pyhäoja, between it and observation tube 210. The confined aquifer is partly artesian in Pyhäoja (see the intermittent spring in Fig. 26). Most of the polluted aquifer is confined, and the polluted groundwater lies below impermeable soil layers. Also marked are the level below which chlorinated phenols (CPs) were found, their concentrations on April 17–24, 1990 (µg l⁻¹) and sampling depth.
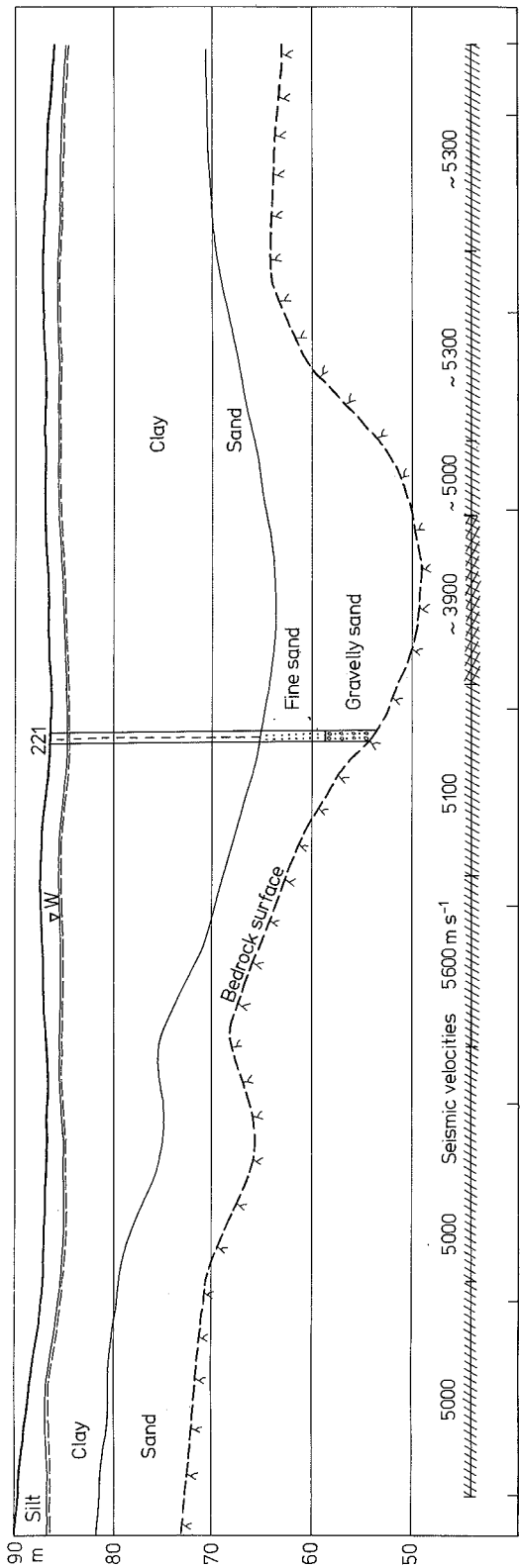
Fig. 28. Cross-section along the same surveying line (9b–8) as in Fig. 26, showing the stratigraphy near the outflow area to be modelled. The overflow at the flowing artesian observation point 221, about 300 m³ d⁻¹, was measured and then stopped on May 18th, 1988.
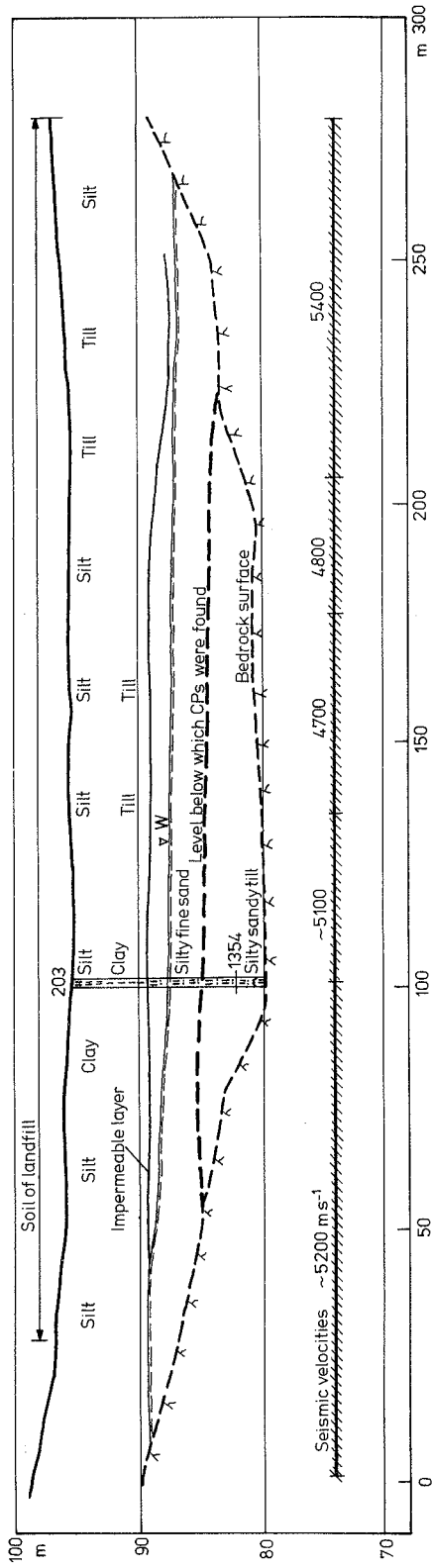
Fig. 29. Cross-section along the same surveying line (6–7) as in Fig. 26, showing the stratigraphy of the bedrock depression. The groundwater heads are based on measurements performed on May 17–19, 1988.

Fig. 30. Locations of drillholes and observations of groundwater head and flow directions (to the Kukonmäki water intake) in the vicinity of the sawmill. Drilling points of known stratigraphy are marked close to the irrigation basins (1–4).

Fig. 31. Stratigraphy of the area surrounding the basins of Ky5 preservative in use from 1957 onwards. Groundwater flows from the basins to observation tube 207 are also depicted.

Fig. 32. Map of sedimentological and geomorphological elements.

Tolkonlähde, and the groundwater in the bedrock depression area also flowed towards Pyhäoja (Fig. 33). After the closure of the Kukonmäki water intake, extraction pumps were operated in its wells for the period 18.12.1987–23.3.1988 in order to stimulate the flow of water, while the water supply in the Järvelä network were ensured via Tolkonlähde until 16.8.1989. Groundwater flow in the area has altered slightly as a result of the closing of the Kukonmäki intake and the temporary increase in extraction from Tolkonlähde. The main direction of groundwater
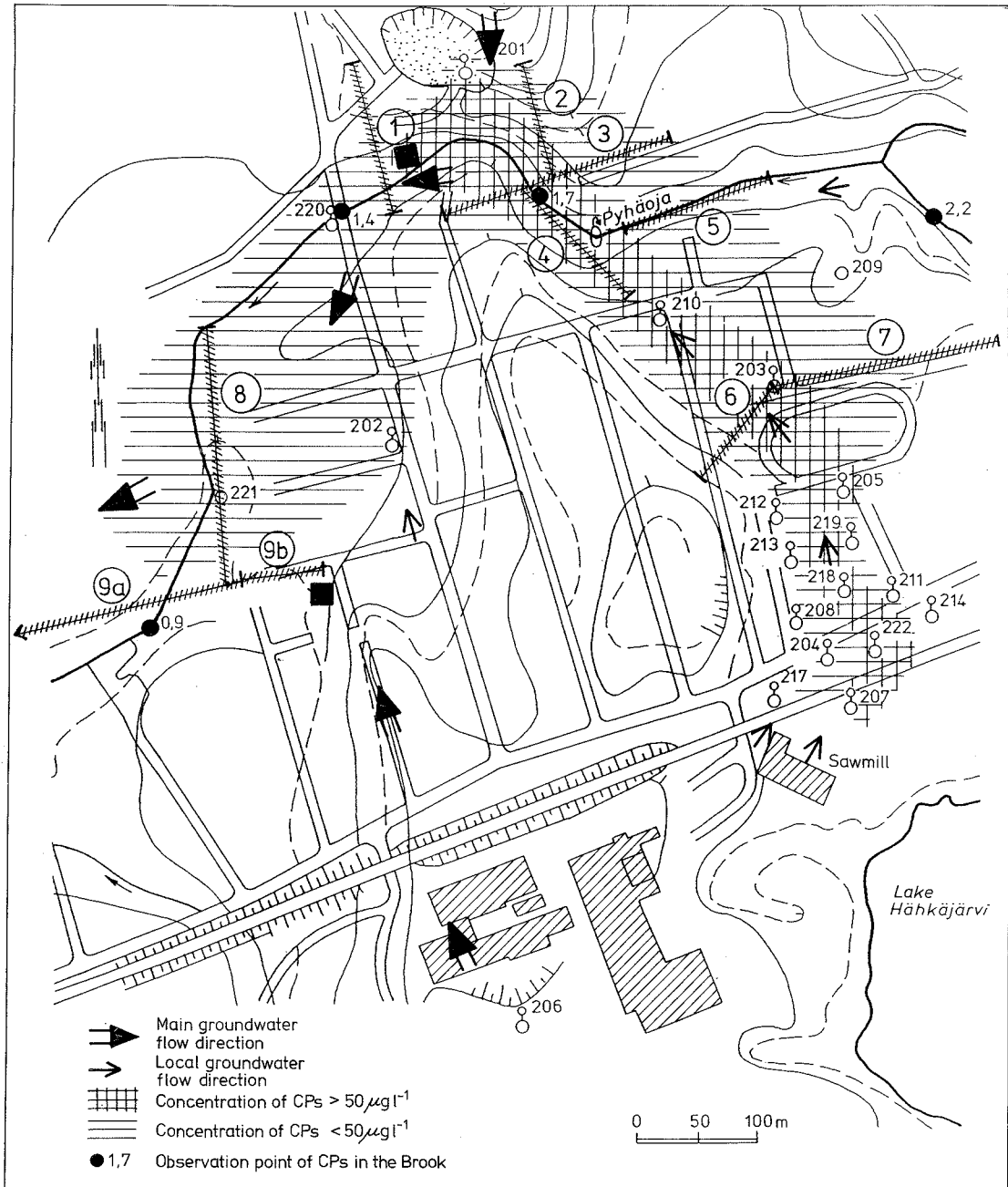
Fig. 33. Concentrations of chlorinated phenols in the groundwater in 1988, and groundwater flow directions in the area modelled.
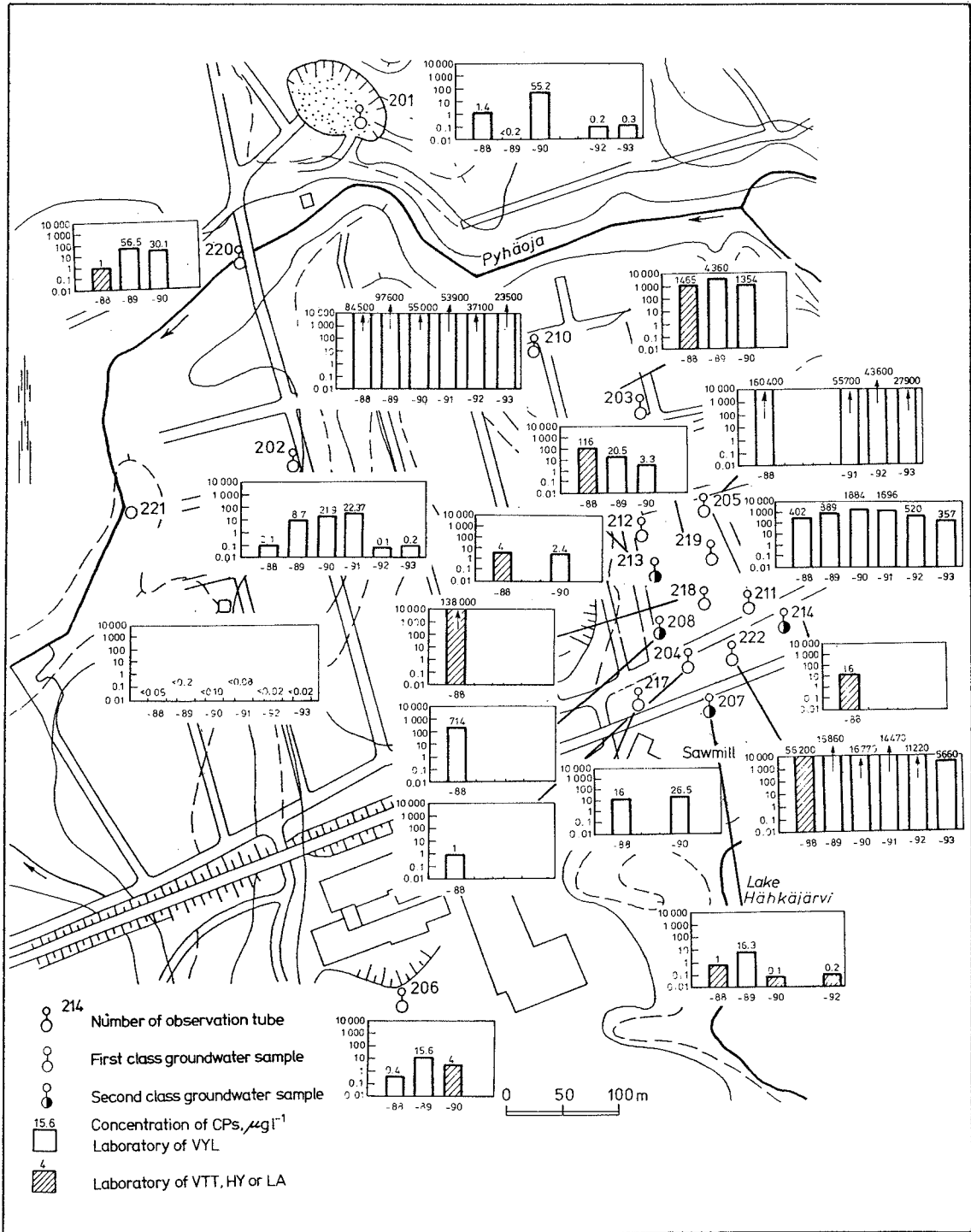
Fig. 34. Concentrations of chlorinated phenols in groundwater samples taken in March and April each year between 1988 and 1992. The analysis results used in the figure are mainly based on those obtained by the Research Laboratory of the Water and Environment Research Institute (VYL), supplemented in the case of missing values with data from the University of Helsinki (HY), the Technical Research Centre (VTT) or the Control and Investigation Laboratory of Lahti (LA).

flow after the closing of the Kukonmäki plant was towards the Pyhäoja valley and Tolkonlähde (Fig. 33).

5.2 Extent of the contaminated groundwater area

Low chlorinated phenol concentrations were recorded in the soil samples taken from near the sawmill and the timber yard, the highest figures being 7.9 mg kg^{-1} in the former area and 6.0 mg kg^{-1} in the latter. Kemtox S10 concentrations of 3.4–16.6 mg kg^{-1} were found in the sawmill area, but none in the groundwater samples.

It was impossible to determine the origin of the chlorinated phenol concentrations observed in the surroundings of the timberyard in 1985, and the geological conditions hampered the detection of groundwater pollution. The timberyard is located on the top of the bedrock ridge, which is overlain by soil layers of thickness from 20 to 30 m, the rock surface sloping away steeply by 20–30 m south-west and south-east of the yard. The soil in the area east of the timberyard is a stony till with occasional boulders and intervening sorted layers. It was difficult to penetrate through the thick soil layers, and the thinness of the groundwater layer and lack of groundwater storage hampered observations of the effects of the emission of chlorinated phenols.

The groundwater samples collected in 1988–1993 were analysed for chlorinated phenols in various laboratories (Fig. 34), with fairly considerable differences in the results obtained (Table 2 in section 4.2). The results presented in Figure 34 are primarily those obtained in the analyses performed by the Water and Environment Research Institute, those produced by the University of Helsinki, the Technical Research Centre of Finland, and the Control and Investigation Laboratory of Lahti being inserted where no results were otherwise available for a given sample. As the water samples collected at different seasons are not directly comparable, Fig. 34 indicates only the chlorinated phenol concentrations in samples taken in spring (March–April). Some of the samples were collected using a tube sampler, but it was not possible to obtain proper samples by this method in every case due to an insufficiency of water in

the tubes. Thus the perched groundwater samples and those obtained with the tube sampler are regarded as 2nd-class samples by contrast with the good-quality, 1st-class groundwater samples, i.e. their representativeness is poor although their results still provide evidence of the occurrence of chlorinated phenols in the groundwater.

The investigations performed in spring 1988 indicated that the groundwater north of the Kukonmäki water intake plant and south of the industrial area was free of pollution. The analyses and the local geology point to transport of chlorinated phenols from the sawmill to the Kukonmäki water intake via the bedrock depression and the Pyhäoja valley, the proportion of highly permeable soil layers increasing from the sawmill towards the sports ground and the Kukonmäki water intake. The highest concentrations were recorded in the deep soil layers lying close to the bedrock surface (Fig. 27).

Groundwater quality monitoring in 1988–1993 pointed to a decrease in chlorinated phenol concentrations in the bedrock depression between the sawmill, the sports ground and Kukonmäki and in Pyhäoja, the contaminated area having spread westwards, following the direction of groundwater flow (Figs. 33 and 34). A slight seasonal variation was observed in the monitoring results, concentrations usually being lower in autumn than in spring (Table 3).

Polluted groundwater seeps into Pyhäoja through the set of springs. According to discharge measurements, e.g. those for October 30th, 1990, there is no overflow of the intermittent spring (Fig. 21) and nor is there any longer any overflow in observation tube 220. The streamflow in the brook itself affects the chlorinated phenol concentrations of the samples obtained from it, as indicated by the fact that the figures for the samples collected in autumn 1991, when the streamflow was low, were on the average higher than those observed at other times (Table 4). Also chlorinated phenol concentrations under detection limit were measured in the brook Pyhäoja from discharge measurement point 0,9 near the modelled outflow area (Fig. 33 and table 4).

The Kukonmäki water intake was closed in December 1987, after which contaminated groundwater was observed in previously unpolluted areas north-east and south of it. This pollution has also spread in the bedrock

depression on account of alterations in flow conditions. The groundwater flowing from the north and north-east tending to push the contaminated water from the Pyhäoja valley towards the south-west. Chlorinated phenols were identified in spring 1990 in the samples collected from observation tube no. 202, representing the area between the Kukonmäki water intake and Tolkonlähde, which had earlier shown no signs of contamination. The groundwater and narrow plume of chlorinated phenols then flows westwards from north-west of Tolkonlähde towards Valkjärvi (see Fig. 16), following the permeable deposits, the gradient of the bedrock surface and possible fracture zones.

5.3 Aquifer properties used to calibrate the groundwater model

The boundaries of the groundwater area and the hydraulic parameters obtained were used to define the initial state for calibration of the MOC model (Fig. 35). The principal input data inserted into the model are listed in Appendix 1. All 528 cells in the grid were assigned input data in the manner illustrated for those in the vicinity of groundwater tubes nos. 203 and 210 in Fig. 36. The parameters and boundary conditions were adjusted so as to ensure that the groundwater heads calculated by the model correspond as well as possible to the measured values. Information

Table 3. Concentrations of chlorinated phenols in observation tube 222.

| Laboratory | Date Depth (m) | Concentration of chlorinated phenols ($\mu g\ l^{-1}$) | | | | |
		2,4,6-TCP	2,3,4,6-TeCP	PCP	Other CPs	Total amounts of CPs
VTT	20.5.1988 15 m	17 000	38 000	1 200	..	56 200
VTT	1.12.1988 13 m	2 800	5 800	2 200	<0.01	10 800
VYL	19.4.1989 13 m	2 200	13 700	960	..	16 860
VYL	17.4.1990 13 m	2 200	14 000	570	..	16 770
VYL	5.9.1990 13 m	1 300	7 000	380	..	8 680
VYL	10.4.1991 13 m	1 600	12 000	870	..	14 470
VYL	2.9.1991 13 m	1 200	7 300	380	..	8 880
VYL	21.4.1992 13 m	1 800	8 900	520	..	11 220
VYL	14.9.1992 13 m	1 700	7 900	470	..	10 070
VYL	20.4.1993 13 m	850	4 500	310	..	5 660

..	= not analysed
CPs	= chlorinated phenols
PCP	= pentachlorophenol
TCP	= trichlorophenol
TeCP	= tetrachlorophenol

Table 4. Concentrations of chlorinated phenols in the brook Pyhäoja.

Laboratory	Date Distance from Lake Valkjärvi (km)	Concentration of chlorinated phenols (µg l^{-1})				
		2,4,6-TCP	2,3,4,6-TeCP	PCP	Other CPs	Total amounts of CPs
VTT	22.11.1988 Pyhäoja 0,9	<0.01	5	14	10	29
VYL	24.4.1989 Pyhäoja 0,9	<0.2	<0.2	<0.2	..	<0.2
VYL	10.4.1991 Pyhäoja 0,9	3.0	16	0.52	..	19.52
VYL	2.9.1991 Pyhäoja 0,9	14	340	17	..	371
VYL	21.4.1992 Pyhäoja 0,9	<0.02	<0.02	<0.02	..	<0.02
VYL	14.9.1992 Pyhäoja 0,9	30	220	13	..	263
VYL	20.4.1993 Pyhäoja 0,9	8.4	33	2.0	..	43.4
VTT	22.11.1988 Pyhäoja 1,4	<0.01	3	<0.01	<0.01	3
VYL	24.4.1989 Pyhäoja 1,4	23	120	4.1	..	147.1
VTT	22.11.1988 Pyhäoja 1,7	<0.01	95	<0.01	14	109
VYL	5.9.1990 Pyhäoja 1,7	230	2 700	92	..	3 022
VYL	10.4.1991 Pyhäoja 1,7	3.5	18	0.56	..	22.06
VYL	2.9.1991 Pyhäoja 1,7	210	1 200	47	..	1 457
VYL	21.4.1992 Pyhäoja 1,7	9.7	42	2.5	..	54.2
VYL	14.9.1992 Pyhäoja 1,7	170	810	43	..	1 023
VYL	20.4.1993 Pyhäoja 1,7	12	46	2.2	..	60.2
VTT	22.11.1988 Pyhäoja 2,2	<0.01	<0.01	<0.01	<0.01	<0.01

.. = not analysed
CPs = chlorinated phenols
PCP = pentachlorophenol
TCP = trichlorophenol
TeCP = tetrachlorophenol
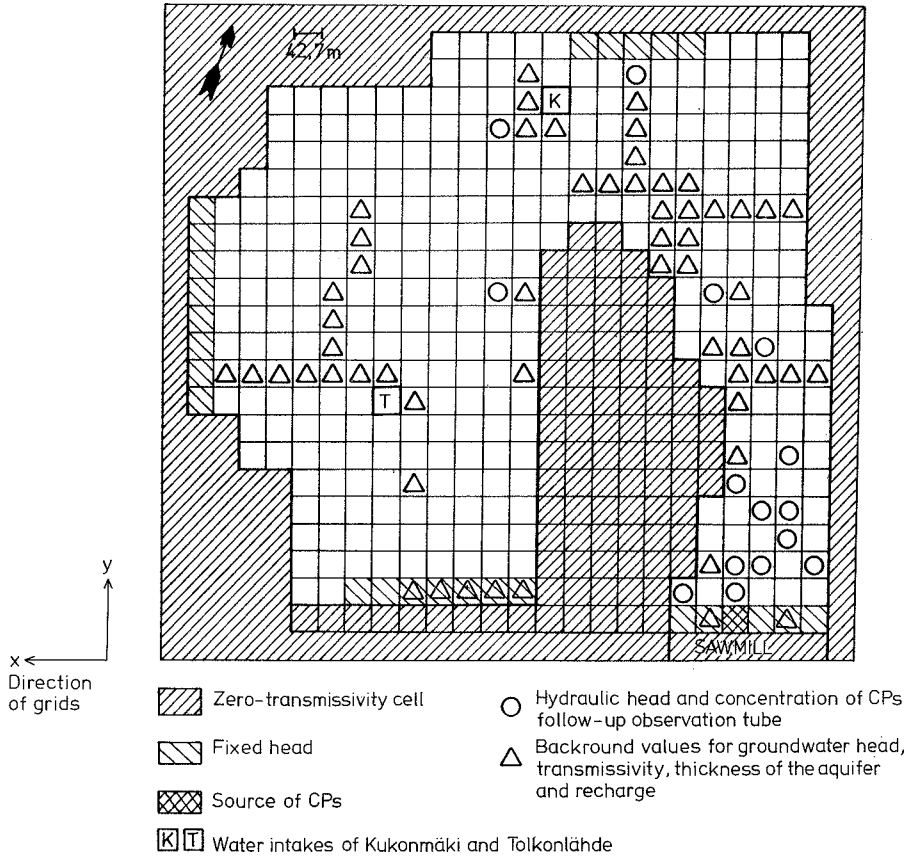
Fig. 35. Node identification in the area modelled.
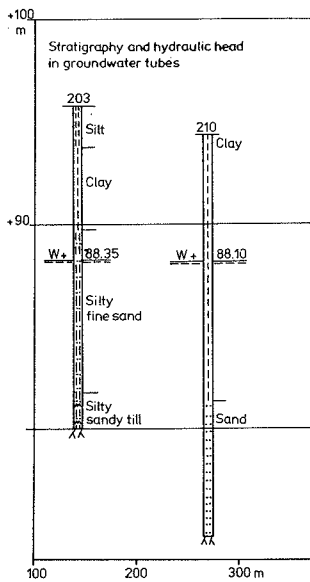
Description of model input data in the model grid area containing groundwater tubes 203 and 210

	203	210
Grid cell	(23,12)	(21,4)
Transmissivity ($m^2\ s^{-1}$)	$9.0 \cdot 10^{-4}$	$2.0 \cdot 10^{-3}$
Thickness of aquifer (m)	6.60	6.60
Concentration at beginning of run (unit)	0	0
Distance of hydraulic head above sea level at the beginning of run (m)	0	0

Calculated heads and concentrations in grid cells (23,12) and (21,14) after of 12 years

	(23,12)	(21,14)
head (m above sea level)	88.61	88.07
concentration (unit)	1	2

Fig. 36. Description of the model input data obtained from groundwater tubes 203 and 210 in steady-state flow (see Fig. 27). The grid description, hydraulic values, time, hydrological, chemical, and execution parameters and program options are listed in Appendix 1.

on the groundwater heads has been collected from a total of 18 groundwater tubes in the area 2–10 times a year since spring 1988, and groundwater table soundings were performed on 10 surveying lines in June 1990 (Fig. 21). Further background information was provided on the hydraulic head of groundwater in the springs, nine private wells and 32 observation tubes in spring 1988. Information on the groundwater heads is presented in the longitudinal and transverse cross-sections of the bedrock depression (Figs. 27 and 29) and in Figs. 28 and 37–39 and Appendix 2. This information was used in the model to mark the boundaries in permeable areas. The model was calibrated by reference to groundwater heads for May 1990, which represent well average levels in a balanced state when the water supply needs of Järvelä had to be met by the Hiidenmäki pumping station, lying outside the area modelled here. The groundwater heads at the boundaries varied from +84.0 m to +93.0 m.

The groundwater area modelled here is primarily a confined aquifer as far as the part affected by the transport of chlorinated phenols is concerned, and the layers with good hydraulic conductive tend to vary in thickness locally (Figs. 32 and 37–38). The average effective porosity is 0.35, the relation between longitudinal and transverse transmissivity (T_{yy}/T_{xx}) 1.0, longitudinal dispersivity 7 m and the ratio between transverse to longitudinal dispersivity 0.5. The above parameters were selected from the literature (e.g. Airaksinen 1978, Freeze and Cherry 1979, Hewett 1986 in Kinzelbach 1991, Bear and Verruijt 1987, Jensen 1988) on the basis of the geology of the area and the final values were determined by calibration. There are two grid cells in the region with pumping wells: those containing the Kukonmäki and Tolkonlähde water intakes.

The groundwater flow is assumed to be steady, the groundwater storage large and seasonal fluctuations in the groundwater head small. The relation between the measured heads remains the same almost throughout the area (Fig. 39). Such fluctuations provide some information on permeability in an area, in that only minor variations occur in highly permeable areas. The groundwater head in the bedrock depression north of the sawmill was found to rise in the periods of high runoff in spring and autumn, while permeability in this area was found to

behave in a manner similar to that of low permeability soils. The depression does not play any significant role in the whole groundwater flow system for the area examined, but it does act as a channel via which chlorinated phenols are capable of entering the highly permeable groundwater area.

It was observed when collecting soil samples from the sawmill area that the perched water formation north of Hähkäjärvi regulates the passage of water into the bedrock depression to enter the groundwater zone. Thus the groundwater heads for May which were used in the calibration represent the average situation, in which water from the perched water storage is flowing into the depression.

Hydraulic conductivity and groundwater recharge were evaluated on the basis of the drillings, seismic soundings and soil type and permeability determinations. The soil of the unsaturated zone was taken as indicative of recharge conditions, the average recharge by precipitation being assumed to be 300 mm a year, excluding the clayey and rocky areas where no infiltration occurs. Infiltration was assumed to be greater than average at the boundaries between permeable and impermeable areas. Recharge inside the modelled area does not play any appreciable role, as groundwater influx at the boundaries of the area was found to be abundant.

The information on the soil of the aquifer was based on samples obtained from the saturated zone. The highest chlorinated phenol concentrations between the sawmill and the Kukonmäki water intake were located in the permeable layers close to the bedrock surface (Figs. 27 and 40). It was in these same contaminated, water-saturated layers that the soils with the highest hydraulic conductivity in the whole profile were located. The highly conductive layers in the saturated zone varied in thickness from 1 m to 30 m in the model.

Hydraulic conductivity and soil type information was collected from the layers which contained the greatest quantities of chlorinated phenols in order to estimate transmissivity. For areas with no chlorinated phenol analyses, the corresponding data were obtained from the stratigraphy of the saturated zone. Hydraulic conductivity was defined for the 11 soil samples, which varied in grain-size distribution from sandy gravel to sandy till, and the hydraulic
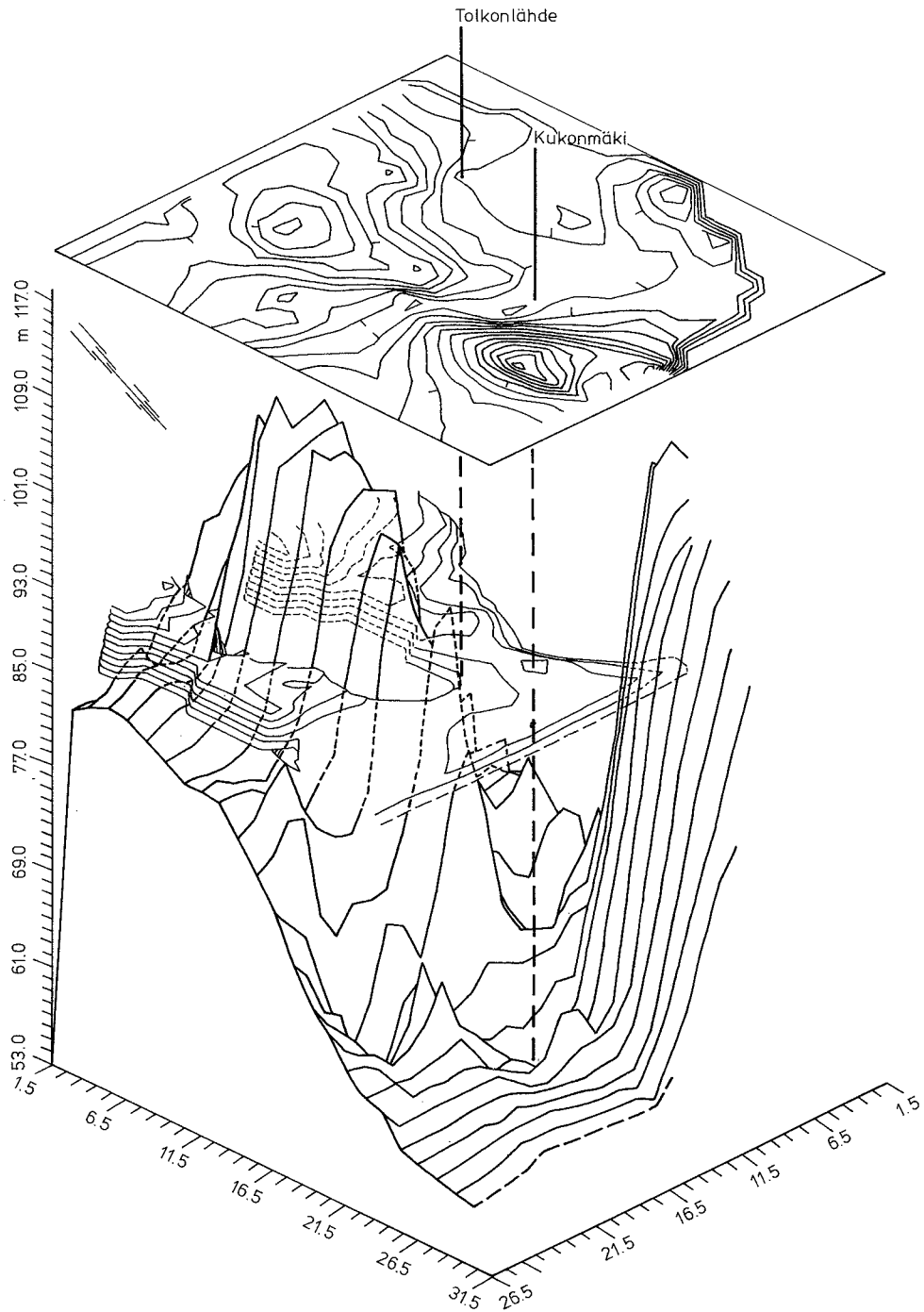
Fig. 37. Three-dimensional model of the bedrock surface (lower surface) and hydraulic head (middle surface) in the area studied. Topographic contour map (upper surface). The unit on the vertical axis is one metre and that on the horizontal axis the number of grids (marked in the middle of each grid).
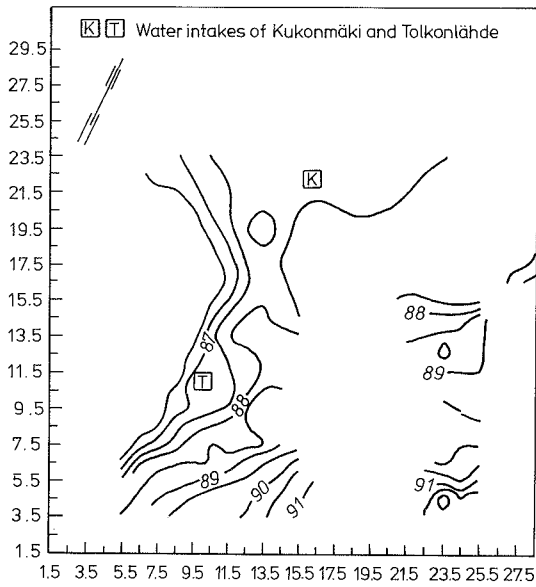
Fig. 38. Smoothed contour map of hydraulic heads in May 1990.

conductivity results, ranging from $1 \cdot 10^{-6.8}$ to $1 \cdot 10^{-2.8}$ m s^{-1}, were compared with both the grain-size distribution of the soils and the mean hydraulic conductivity values given for various soil types in literature (see Fig. 2). Eventual transmissivity values ranging from 0 to $3 \cdot 10^{-2}$ m^2 s^{-1} were determined by calibration (Fig. 41).

Groundwater was pumped into Pyhäoja from the contaminated Kukonmäki water intake during the period 18.12.1987–23.3.1988, i.e. after the closure of the latter, while some of the water required by the village of Järvelä was supplied from Tolkonlähde until 16.8.1989. This increased extraction from Tolkonlähde did not eliminate the overflow, which was still 100–200 m^3 d^{-1} in the spring. Overflow in the spring had varied from 1 000 to 1 500 m^3 d^{-1} in the 1970's and 1980's, when mean annual extraction at the Kukonmäki water intake was in the range of 484–1 005 m^3 d^{-1}. Average monthly pumping volumes for 1986 and 1987 are shown in Fig. 42.
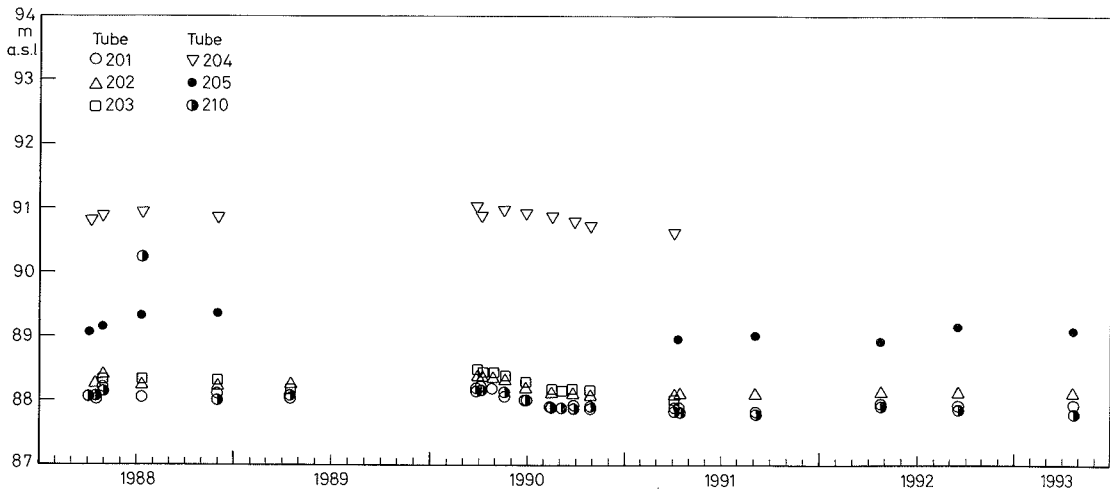
Fig. 39. Hydraulic heads in the six observation tubes between April 6, 1988 and April 20, 1993.

Under prevailing conditions, the polluted groundwater is advancing in the form of a narrow zone in the village of Järvelä. The model was not calibrated with respect to the concentrations, as chlorinated phenols had already been released into the groundwater for some tens of years (Lampi et al. 1992) and no information was available on the exact times of such releases nor on the chlorinated phenol concentrations at the site of release. The data on the chlorinated phenols were thus inserted into the model on the assumption that these entered the groundwater in the form of a single emission in the source cell,

situated on the boundary between the modelled area and the sawmill. The recorded concentrations were nevertheless used as incidental tracers for the modelling of the flow and the relative dilution of the chlorinated phenols.

The transport of chlorinated phenols in the groundwater was modelled as in worst-case scenario analysis, assuming that no reactions or adsorption took place. This approach is justified by the fact that chlorinated phenols are permanent under the groundwater conditions prevailing in Finland (Valo 1990).
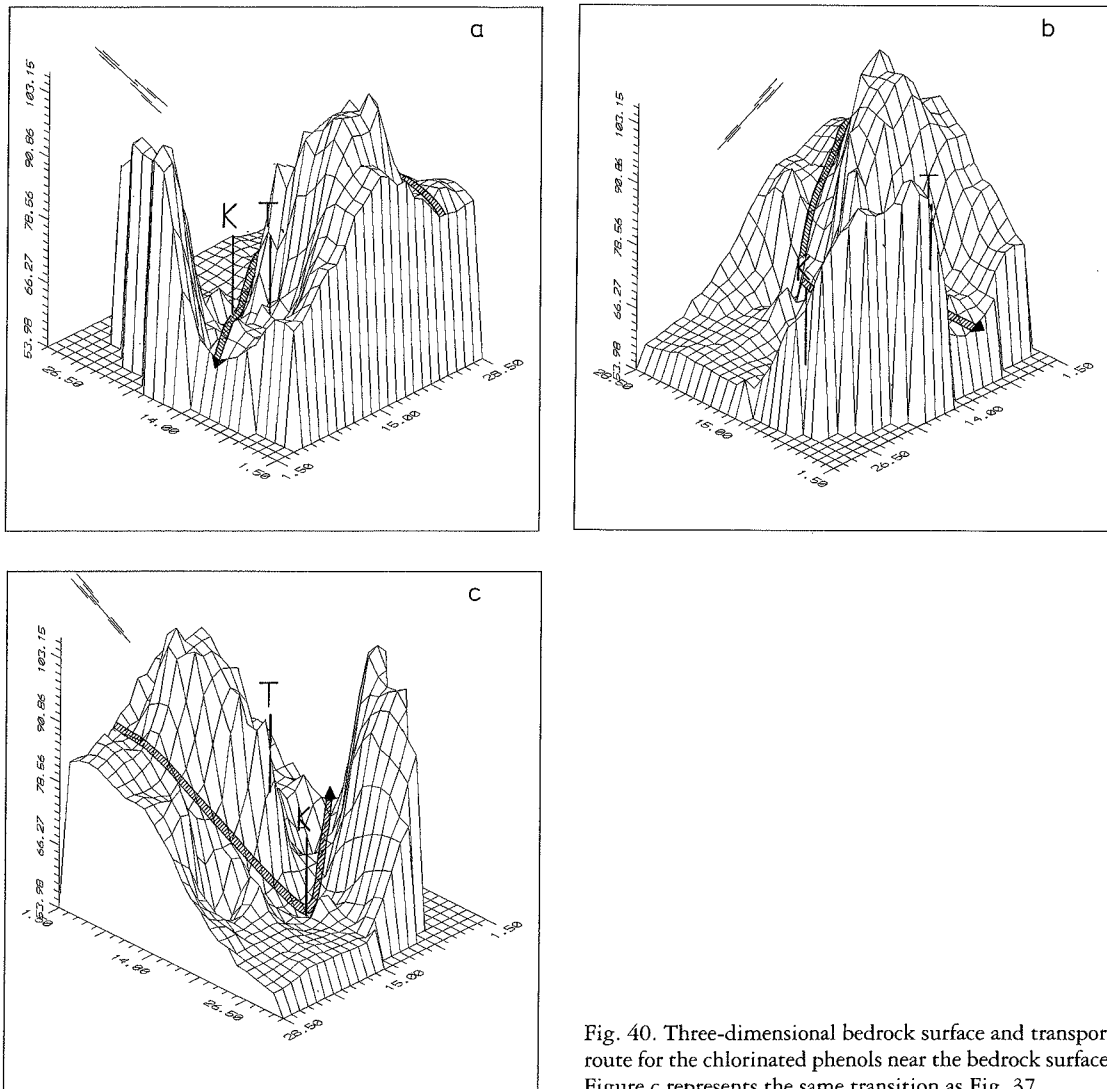
Fig. 40. Three-dimensional bedrock surface and transport route for the chlorinated phenols near the bedrock surface. Figure c represents the same transition as Fig. 37.

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T value (m²s⁻¹)

0

$1 \cdot 10^{-5} \leq$ $< 5 \cdot 10^{-5}$

$5 \cdot 10^{-5} \leq$ $< 9 \cdot 10^{-5}$

$1 \cdot 10^{-4} \leq$ $< 5 \cdot 10^{-4}$

$5 \cdot 10^{-4} \leq$ $< 9 \cdot 10^{-4}$

$1 \cdot 10^{-3} \leq$ $< 5 \cdot 10^{-3}$

$5 \cdot 10^{-3} \leq$ $< 9 \cdot 10^{-3}$

$1 \cdot 10^{-2} \leq$ $< 2,5 \cdot 10^{-2}$

$2,5 \cdot 10^{-2} \leq$ $\leq 3 \cdot 10^{-2}$
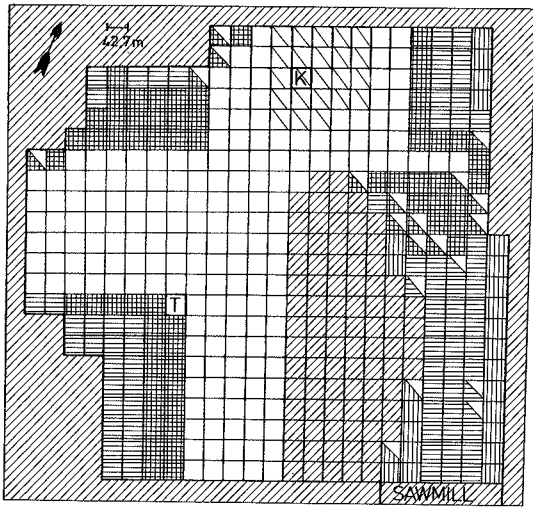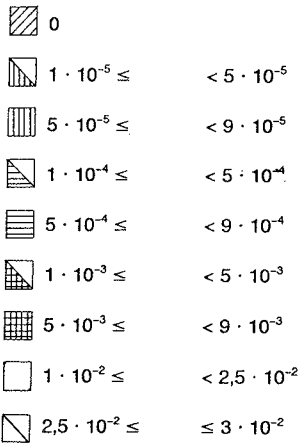
Fig. 41. Averaged transmissivity map.
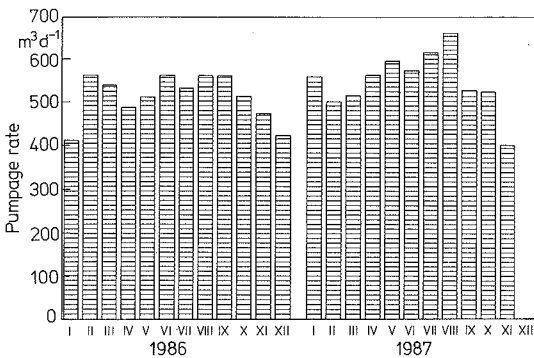
Fig. 42. Average monthly pumping rate at Kukonmäki in 1986 and 1987.

6 DISCUSSION

6.1 Flow modelling

Flow conditions in the area were simulated for the situation in which the Kukonmäki water intake was pumping normally (Fig. 43), employing the mean intake rate for the period 1981–1987 of $572 \ m^3 \ d^{-1}$. The calculated heads (depicted at half a metre intervals) nevertheless did not differ much from those prevailing under the present conditions (Fig. 44). Examination of the individual nodes in the grid showed that the gradient in the groundwater head in the area between the sawmill and the Pyhäoja valley was greater when the Kukonmäki water intake was in
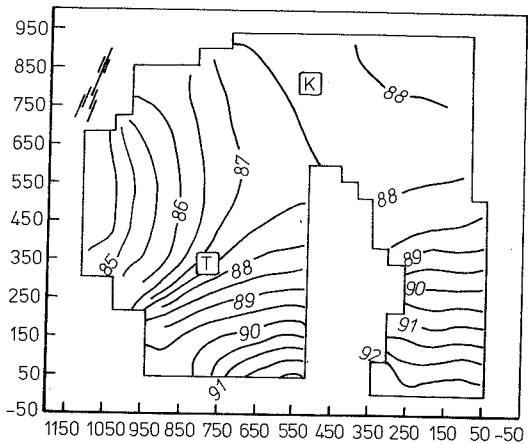
Fig. 43. Computed hydraulic heads when the pumping rate at the Kukonmäki water intake is $572 \ m^3 \ d^{-1}$. The contour interval is half a metre.
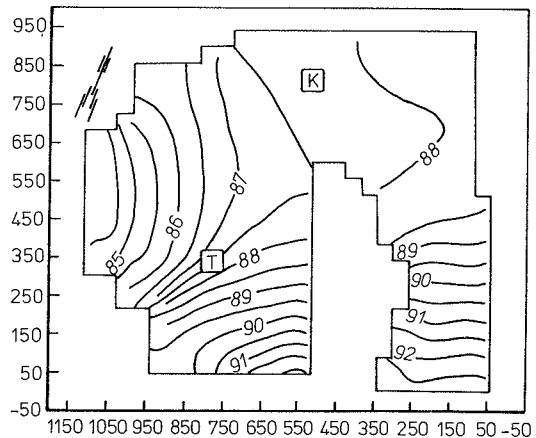
Fig. 44. Hydraulic heads computed by means of the calibrated model.

use than when it was not, and that in the latter case there were only minor variations in water head between Tolkonlähde and Kukonmäki, because the area is highly permeable. Finally, in spite of the location of the constant head boundary in the Kukonmäki esker area to the north of the Kukonmäki water intake, the simulation results indicate that pumping at the Kukonmäki water intake also slightly increases the gradient in the area south of the Kukonmäki water intake.

The mean groundwater heads for the area studied, when calibrated to correspond to the given flow conditions, do not match the measured values everywhere (Figs. 44 and 38), because the two-dimensional model does not allow soil layers of differing hydraulic conductivity to be taken into account and admittedly the isopotential curves based on the measurements of groundwater head do not contain enough data points for the area north of the Kukonmäki water intake. The calibration could not be fixed with reference to the situation in which this water intake was in use or with reference to the pumping of polluted groundwater during the period 18.12.1987–23.3.1988 because the installation of permanent groundwater tubes began only on the day on which the pumping ceased.

6.2 Transport of chlorinated phenols

The spread of pollution under steady-state conditions after closure of the Kukonmäki water intake is illustrated in Fig. 45 in which it is assumed that pollution occurred in a single emission and that transport of chlorinated phenols in the bedrock depression takes place constantly throughout the year. One occasion of pollutant release of this kind would have been the fire that occurred at the sawmill on 19.5.1976. The grid square containing the sawmill site itself was assigned a chlorinated phenol concentration of 1 000 units. The mean pumping rate at the Kukonmäki water intake, 572 m³ d⁻¹, corresponds to a situation in which polluted water is flowing towards it throughout the year (Fig. 46).

After a simulation period of 12 years the whole area examined here is seen to have a pollutant
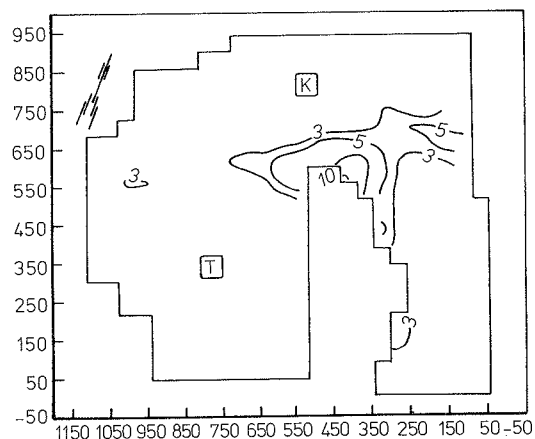

Fig. 45. Calculated plume following a single emission of chlorinated phenols while the Kukonmäki water intake is closed, assuming a steady-state flow over 12 years. The source concentration at the sawmill is taken as 1 000 units, the discrimination limit for chlorinated phenols on this contour map is three units and the other levels are 5, 10 and 15 units.
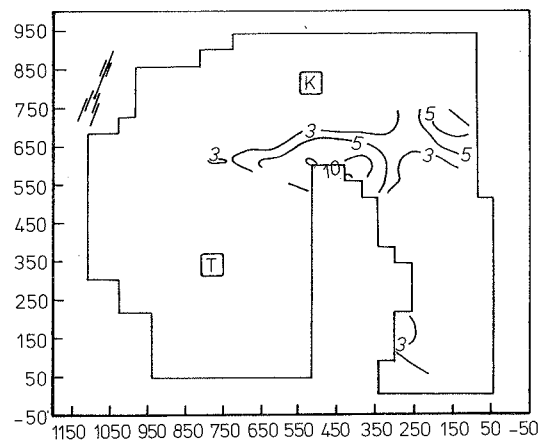
Fig. 46. Calculated plume following a single emission of chlorinated phenols while the Kukonmäki water intake is functioning at a rate of 572 m³ d⁻¹, the average for 1981–1987, assuming a steady-state flow over 12 years. The source concentration at the sawmill is taken as 1 000 units and the discrimination limit for chlorinated phenols is three units.

concentration of 1–16 units, regardless of whether the Kukonmäki water intake is in use (intake 572 m³ d⁻¹) or not (Figs. 45 and 46), and even after 6 years the pollution plume in the aquifer is seen to have advanced from the bedrock depression to the Pyhäoja valley. Its advance

towards the outflow area of the grid modelled proceeds slightly more slowly when the Kukonmäki water intake is in use, and the plume is slightly narrower and more continuous. The modelling results (Figs. 45 and 46) clearly demonstrate that many decades will elapse from the removal of the source of pollution before the aquifer in the area is cleaned by natural groundwater flow. Measurements show that the polluted groundwater is advancing through the soil all the time, and is also being discharged at the springs and ditches, passing along the brook Pyhäoja towards Lake Valkjärvi.

6.3 Reliability of the modelling results

6.3.1 The MOC model

There are two means of reducing the uncertainty attached to a groundwater model. One can either choose a more detailed model for the region concerned, usually by including another dimension or allowing for processes or dynamics that had previously been ignored, or else one can collect more data, which is perhaps the more common approach (Peck et al. 1988, p. 138). The two-dimensional MOC model was employed here because one aim of the work was to test its suitability for the modelling of a small heterogeneous aquifer, and the initial data consisted for the most part of material gathered for monitoring purposes. No separate resources were available for this research, but rather the modelling and the additional research required for it were carried out according to the opportunities that became available in the course of normal working routines at the Water and Environment Research Institute.

The MOC model is a reliable numerical groundwater model involving a computer program constructed to provide approximative solutions based on mathematical regularities to equations describing flow and solute transport conditions in a given area (e.g. Beljin and van der Heijde 1989). The use of numerical programs requires a thorough knowledge of the model concerned, for as Heijde et al. (1988) point out, the solution of a modelling problem entails recognition of the limitations attached to the model and the equations on which it is based. The MOC model assumes a confined aquifer system (see remarks on the equations and limitations of the MOC model in section 4.3.2), although de Marsily (1986) claims that the equations derived for a confined aquifer can also be applied to an unconfined one provided that the change in groundwater head is not more than 10 % of the thickness of the saturated zone. This is the case in the unconfined areas of the present aquifer.

6.3.2 Input data for calibration

The modelling process calls for a clear qualitative and quantitative conceptual model, and it is obvious from post-audits reported in the literature that "a valid and complete conceptual model is essential for making accurate predictions" (Anderson and Woessner 1992). Since a model simulates situations which cannot be verified experimentally or which apply only to the future, it is only careful definition of the problem and adequate expertise on the part of the user of the model that can guarantee that the method will be implemented correctly.

The need to select meaningful boundaries may require the modelling of a large area (Anderson and Woessner (1992), and the size of the area will in turn affect the selection of the interval between the nodes. A grid with a small number of nodes is preferable in order to minimize data handling and computer storage and computation time. Anderson and Woessner (1992) concede that initial properties such as recharge rates may change significantly from one cell or element to another, but it is typical for there to be few field measurements of recharge rates available, so that a constant value is usually assumed over a large portion of the grid. The geological properties of heterogeneous aquifers in Finland, of the kind represented by the Järvelä area, can vary considerably from one cell to the next. As the main emphasis here was on the geology of the area, the modelled area of 1 km^2 was divided into 624 cells, of which 83 were deemed to represent the bedrock of the watershed area. Measurement data are available for 59 cells which represent the porous medium of the area (Fig. 35). The density of cells and data points is high relative to the other documented applications of the model to the transport of pollutants in porous media

published for Finland (Ahlberg et al. 1988, 1991; de Coster et al. 1993, Granlund et al. 1993).

Even when large amounts of data are available, the boundary conditions and properties of the aquifer always involve elements of uncertainty. Modelling is impossible without reliable sources of data, because the accuracy of the results is proportional to that of the data and has an effect on the eventual outcome. Some of the present data were collected for supervision purposes before the pollution had been discovered or before groundwater modelling had commenced, and not all the data are directly usable for calibrating the model, although everything that can be recorded is valuable as background information for formulating a picture of the geology of the area and in this way can be made use of when evaluating the reliability of the modelling results.

It is essential that the data should be representative of the area to be studied. Anderson and Woessner (1992), for example, postulate that heads and fluxes should ideally be measured at large numbers of locations uniformly distributed over the region being modelled. Unfortunately geological factors often prevent one from obtaining all the initial data which would in theory be necessary, and the remainder have to be estimated by interpretation and interpolation from the known facts and via calibration of the model. Parameters in the model that are defined by calibration are the more reliable the less variables have to be estimated. Calibration by trial and error is a flexible method, particularly when the quantity of source data is limited.

Although many eskers are known to have accumulated in fracture zones, it remains unclear from the present research whether the depression marked by the Pyhäoja valley is a consequence of bedrock fracturing. A transverse seismic sounding transect to the north of the Kukonmäki water intake would perhaps have helped to show whether there is any fracture zone or not, but no soundings were carried out across the esker in the present programme on account of the variations in topography and the depths of the overlying loose deposits. Groundwater modelling as such is an effective tool for studying the presence or absence of fracture zones in bedrock, as it is difficult to match the measured and modelled groundwater heads at the calibration stage, even though the calibration may be based on accurate hydraulic conductivity and groundwater head

data for the porous medium, if the base of the model for the area leaks or lets water in. Calibration of the present model did not reveal any fracture zones in the Pyhäoja area. Anderson and Woessner (1992) emphasize the importance of recognizing that a specified head boundary represents an inexhaustible supply of water, and that a groundwater system may pull water in from such a boundary without altering the head at all at the node in question. As the northern part of the esker modelled here acts as a constant head boundary, this in itself will prevent the accurate demonstration of any fracture zone in the Pyhäoja valley.

Effective porosity does not have any great effect of the dissemination of the pollutant in this application of the model, and thus no separate calibration was performed to account for it. It is also inherent in the assumptions of the MOC model that no chemical reactions occur that affect the concentration of dissolved substances, the fluid properties of the water or the properties of the aquifer. In practice the chemical reactions typically used in transport models are limited to adsorption, described by a retardation factor, and hydrolysis and decay, described by a first-order rate constant (Anderson and Woessner 1992). There was no need to consider adsorption in the present worst-case scenario analysis.

One confounding factor when attempting to quantify dispersion is the 'scale effect', by which dispersivity seems to increase with the size of the contaminant plume (Freeze and Cherry 1979, Marsily 1986), or as the plume moves down the gradient (Anderson and Woessner 1992). Dispersion values taken from the literature were tested here and the final figures were determined by calibration. It was unreasonable in this case to attempt multistage calibration of the dispersion coefficient, as the distribution of chlorinated phenol concentrations in the area is markedly three-dimensional and the emission dates and rates are unknown. According to Anderson and Woessner (1992), it has been customary to estimate dispersivity by means of trial and error calibration of the model and with tracer tests. Consideration of transport in an anisotropic porous medium may require estimation of more than two parameters, i.e. vertical as well as longitudinal and transverse dispersivity (Konikow 1991). There are nevertheless many aspects of the transport and dispersion of solutes

in anisotropic porous media that are still poorly understood (see Peck et al. 1988, Konikow 1991, Anderson and Woessner 1992).

The installation of groundwater tubes at low-lying sites at Kärkölä caused the discharge of confined groundwater contaminated with chlorinated phenols and at the same time altered the groundwater flow conditions. The result was that it became necessary to block off the pipe on the western edge of the area to be modelled as soon as it was in place (no. 221 in Figs. 26 and 28). Similarly the water was found to rise above ground level in the westernmost groundwater observation tube (no. 220 in Fig. 26) until it had sought out new flow routes following the closure of the water intake, the installation of the tubes and the ditching carried out in the Pyhäoja valley. The flow field of the surroundings of the Kukonmäki water intake in the Pyhäoja valley remained variable for some time, until the flow conditions in the aquifer regained a steady state. Thus the installation of observation tube no. 220 caused the overflow at the Kukonmäki water intake to cease, although some overflow still takes place at the tube itself when spring and autumn runoff reaches unaccustomed volumes.

The hydraulic conductivity properties of the aquifer had to be estimated and calibrated, as measurement data were not available for the whole area. The individual measurements represent only local conductivities at certain observation points, whereas the data inserted into the model represent mean regional properties. Groundwater flow velocity measurements performed in the field would have provided for more accurate estimation of transmissivity. On the other hand, the large amount of information available on soil types in the area was of considerable significance for the determination of average hydraulic conductivity properties for calibration purposes.

Unfortunately it was not possible to obtain a continuous series of groundwater head measurements distributed evenly over the area in order to calibrate the model, and the individual accurate readings that were available represent in reality only the geology of the observation points themselves. The values assigned to a grid are in general mean properties of the aquifer in the cells concerned, and in reality all aquifers are three-dimensional, with the local soils, their stratigraphy and their hydraulic conductivities capable of varying significantly. This was true of the present aquifer, where the sediments of the bedrock depression deviated in their properties from the rest of the aquifer, e.g. they were of lower porosity, but the MOC model allowed only one porosity value to be assigned to the whole modelled area.

Specified head conditions should be selected whenever possible in groundwater modelling rather than specified flow, because the former is easier to measure (Anderson and Woessner 1992), and it is for this reason that the volumes of water flowing into the area were not used as boundary conditions. The overflow from the Tolkonlähde water intake and seepage springs was measured (see section 4.1.3), and groundwater yield surveys (Insinööritoimisto Paavo Ristola Oy 1973, Helsinki Water and Environment district 1988) were used to evaluate the reliability of the results calculated by the model. No pumping tests were performed, because these would have brought about changes in the groundwater flow conditions and caused the pollution to spread over a wider area or generated a large quantity of problem waste in the form of the water pumped out. Similarly any attempt at purifying the aquifer by pumping off the contaminated groundwater would have yielded vast quantities of liquid akin to the original Ky5 impregnation solution, which is difficult to treat by the methods currently available for problem waste of this kind.

The decision to treat the groundwater flow here in terms of a steady-state model was justified, as seasonal variations in the groundwater head are small. The modelling of transient flow would require determination of the storage coefficient, and this in turn would call for the use of pumping test results, none of which were available in the present case. The modelling of seasonal changes would also require accurate monitoring data on the recharging of groundwater reserves.

Similarly the examination of the dilution of the chlorinated phenols assumes a situation in which the perched groundwater north of Lake Hähkäjärvi washes the substances out and transports them away at a constant rate regardless of the season of the year. The groundwater head monitoring data indicate that more perched groundwater than usual flowed into the bedrock depression in spring 1988, but no measurements of this effect are available for the time preceding

the discovery of the pollution. Again this assumption of a constant rate of water inflow into the bedrock depression does not affect the mean flow routes or transport routes for the pollutant plume, and as the inflow of water into the modelled area from elsewhere is large, the assumption is not of any great significance as far as flow volumes in the area as a whole are concerned.

Other minor factors capable of affecting transport routes are the small springs, the ditching carried out in the Pyhäoja valley, pumping at the Kukonmäki water intake before and after its closure. The continuous pumping of water at the Kukonmäki intake prior to the discovery of the pollution may have extracted the pollutant from the bedrock depression in a manner different from that prevailing in the calibration situation, when the water intake was closed. Also, the occasional sprinkling of the logs in the timberyard to keep them moist in dry weather may have caused unknown amounts of water to infiltrate into the soil, while yet another unknown quantity is the spread of chlorinated phenols in an east-west direction during periods when there is an exceptionally low rate of flow into the bedrock depression.

6.3.3 The calibration process

Qualitative and quantitative error

Although not all the source data inserted into the model were direct measurements, some being acquired from the literature or through calibration, the calculated groundwater heads for May 1990 corresponded fairly well to the measured ones (Figs. 37 and 39, see also Figs. 38 and 44 and Appendix 2). The extent of the modelled plume of pollutant also corresponded to the pattern of measured chlorinated phenol concentrations (Figs. 33, 45 and 46). Thus the differences between the measured and calculated groundwater heads over the whole area vary from zero to 1.30 m. For example, the simulated groundwater tables of +88.07 and +88.09 m for the cells containing observation tubes 210 and 201 correspond extremely well to the measured values of +88.10 and +88.09 m. The mean difference between the measured and simulated heads in the modelled area (mean error) is −0.18

m and the mean of the absolute values of the differences (mean absolute error) is 0.62 m. The greatest discrepancies are found in the area of the bedrock depression occupied by the pollution plume, where hydraulic conductivity around the observation tubes is poor and the heads vary significantly from one season to another or groundwater occurs only sporadically. The mean error in the bedrock depression is −0.42 m and the mean absolute error 0.70 m. Att the local variations in hydraulic conductivity occurring in the area of the bedrock depression were not inserted in the model as the program cannot cope with the calculations when the transmissivity values fluctuate greatly between adjacent nodes in the grid. It is for this reason that the contiguous zone penetrating the area from east of the bedrock watershed (tube 212 in Fig. 33) cannot be recognized as impermeable. This homogenization of the initial data for modelling purposes has the effect of yielding slightly exaggerated flow and transport velocities.

Water and mass balance in the calibrated model

The calculated total rate of flow through the area in the calibrated application of the model is approximately 0.06 m^3 s^{-1} (=2.12 ft^3 s^{-1}, Appendix 3). It is significant that the error in the water mass balance in this case is less than 0.01 %, and the mean error in the chemical mass balance of is 5 %. According to Konikow and Bredehoeft (1984), an error in mass balances is acceptable if it is less than 10 %. The calculated flow rate is higher than the estimated real flow rate, because this is a worst-case scenario analysis and the real aquifer is highly three-dimensional with respect to its hydraulic conductivity and porosity values.

Sensitivity analysis

The sensitivity of the model was tested with the parameters inserted into the model as a result of the calibration, i.e. groundwater heads at the boundaries, initial parameters and distributions of parameters such as transmissivity throughout the area. The model proved to be sensitive to the transmissivity and boundary values inserted into

it, the last of these being the most susceptible source of error, in that if the boundary values are incorrect the whole flow field will be calculated wrongly. According to sensitivity analysis a constant head boundary 8–10 cm higher than the true value at the edge of the Kukonmäki esker will cause an increase of about 6 cm in the predicted groundwater table at the Kukonmäki water intake and 1.5 cm in that at Tolkonlähde relative to the calibration situation, the corresponding figures for a 0.5 m excess in the constant head boundary being 0.43 m and 0.11 m respectively. Also, if the boundary conditions are not realistic, the transmissivity determined by calibration and the predictions calculated by the model will be erroneous. Not even precisely measured hydraulic conductivities will suffice to provide reliable predictions if incorrect groundwater heads are inserted in the model as boundary conditions.

The sensitivity of the model to transmissivity was tested over the whole area by employing values which were ten times greater and smaller than those used in the calibration. Peck et al. (1988) postulate that when calibrating a model by trial and error with respect to the hydraulic head, the range of variation in transmissivity should be determined node by node or area by area. When this was done in the present sensitivity analyses for variations in transmissivity, errors were apt to appear in the groundwater heads, the error in water balance increased and the model collapsed at the stage of calculating transport at the latest. Locations that proved particularly sensitive to changes in transmissivity were the edges of the bedrock area in the centre of the area modelled.

The use of transmissivity values which were one tenth of those used in the calibration led to a major discrepancy in groundwater heads relative to the measured ones, the values given by the model being higher than the measured ones in the bedrock depression area and lower in the esker area. The largest discrepancy was 7.58 m, in the vicinity of Tolkonlähde. These test calculations suggested that over the same period as was required for the chlorinated phenols to travel to the outflow area in the calibrated model, i.e. 12 years, they would be transported no more than 150 m.

The groundwater heads obtained with transmissivities ten times greater than those used

in the calibration corresponded fairly well to the measured values, having a mean error of 0.78 m and a mean absolute error of −0.37 m. The transport times, on the other hand, are utterly unrealistic, suggesting that the tip of the chlorinated phenol plume would reach the water intake in less than a year and the outflow area of the model in about a year. Thus there would be few remains of the pollution in the Pyhäoja area two years after a single emission and none after four years even in the recesses of areas with the most difficult flow conditions. This may be compared with the calibration situation, in which it is estimated to take 12 years for the tip of the plume to reach the modelled outflow area, and the actual situation, in which measurements show that 12 years after the fire in the sawmill chlorinated phenol concentrations in the groundwater over an extensive part of the modelled area corresponded to the strength of the Ky5 solution used for impregnation. The chlorinated phenols serve here as an unintentional tracer substance, and their distribution lends precision to the evaluation of the reliability of the transmissivity values.

6.3.4 Evaluation of the modelling results

The equations contained in the MOC model are based on the assumption that vertical variations in hydraulic head and pollutant concentration are minimal and the only force giving rise to flow is derived from gradients (Konikow and Bredehoeft 1984). Part of the aquifer modelled here is unconfined and part is confined, and the alternation between these classes, together with the bedrock surfaces and the lower surfaces of the thick clay beds are forces that affect the flow conditions. If one examines only the groundwater heads, the bedrock surface and the variations in the thicknesses of the clay beds overlying the aquifer (Figs. 27, 33, 34 and 39) have directed the chlorinated phenols to flow 'upstream', towards tubes 201 and 202. And if we compare only the hydraulic heads in the tubes installed at low-lying sites, the variations in groundwater table calculated by the model, and indirectly also the variations in the thickness of the aquifer, are evened out relative to the behaviour of the actual aquifer. In order to keep the direction of flow correct, the smoothing of the actual differences in

gradient between the hydraulic heads has been corrected in the course of calibration. The transmissivities are calibrated so that the head gradient differences in the esker area (Tolkonlähde, the Kukonmäki water intake and groundwater tubes nos. 201, 202 and 220) and in the bedrock depression (e.g. groundwater tube no. 210) are correct relative to each other.

It is assumed in the MOC model that the flow is horizontal, i.e. it has no vertical component (Konikow and Bredehoeft 1984), but this assumption falls down in regions where the actual flow has a large vertical component, e.g. in the vicinity of an outlet (water intake, spring, etc.). As a simple rule, the flow must be taken to be three-dimensional at distances less than 1.5 to 2 times the thickness of the aquifer (Bear 1979). The groundwater heads calculated by the model, even when plotted at half a metre intervals, illustrate the manner in which a change in pumping at the Kukonmäki water intake will affect the heads in the Pyhäoja valley in the northern part of the area (Figs. 43 and 44). In reality, pumping at the water intake does not have any major impact on nearby heads, on account of the constant head boundaries north of the Kukonmäki water intake, and the huge highly permeable groundwater reserves in the area to the north of the water intake ensure that the constant head found there is an acceptable boundary condition.

Since the overflowing spring at the Tolkonlähde intake was treated as a water pumping cell in the model, its discharges are envisaged, contrary to fact, as lowering the head in and around the spring cell. The model was also used to test the effect of a number of small springs in the Pyhäoja valley discharging polluted water, but the effort was abandoned as heads were predicted to drop over a disproportionally large area of the Pyhäoja valley and the bedrock depression, again departing from the real situation. The seepage from the springs is in fact very small relative to the water balance of the whole area.

Regardless of whether the Kukonmäki water intake is functioning or not, the chlorinated phenols will flow past to the south of it under mean flow conditions, and none have been observed at it since the installation of the overflowing groundwater tube 220 in spring 1988. Discrepancies between measured and modelled distribution of a pollutant are possible even in small areas, as the model does not take account of differences in hydraulic conductivity in a vertical direction between the soil layers.

It is not recommendable, on the other hand, to make detailed comparisons between modelled and measured chlorinated phenol concentrations, as the application of the model does not take account of all the factors affecting their transport. In the first place, it sets out from the assumption of a single emission of the pollutant into the system, whereas in the reality it was released on a number of occasions (Lampi et al. 1992), although we do not know the exact dates nor the quantities involved. Thus the modelling of their transport is more a matter of tracing the routes by which this took place than of calculating individual concentrations.

Calibration of a model of this kind requires a sufficiently long series of observations with which the results obtained from the model can be compared. In the present case the groundwater head measurements performed in 1988–1990 were not used for calibration purposes because the area had undergone a number of changes by that time which would have altered the groundwater flow, e.g. groundwater pumping, installation of the observation tubes and the ditching in the Pyhäoja valley. This means that, in view of the absence of any series of accurate hydrological measurements for the period preceding the pollution of the groundwater, this calibrated model cannot serve as a reliable means of simulating either the times of pollution or flow conditions prior to the steady-state flow pattern achieved in spring 1990. On the other hand, it is applicable to a restricted degree to the prediction of transport routes for the polluted groundwater and of groundwater heads under various sets of groundwater pumping conditions (see sections 6.1 and 6.2). The eventual reliability of any prediction of the effects of cleanup pumping will become apparent only when it is possible to assess whether the situation modelled has come into being in reality.

7 SUMMARY AND CONCLUSIONS

A sawmill located at Järvelä in the municipality of Kärkölä in Finland was placed under

surveillance because the wood preservative Ky5, the main components of which are trichlorophenol, tetrachlorophenol and penta-chlorophenol, was known to have been used there from the 1930's until 1984. Pollution of the water intake 800 m from the sawmill was observed in December 1987, its chlorinated phenol concentrations exceeding the maximum permitted by the National Board of Medicine, 10 μg l^{-1}, by a factor of ten, and the facility was closed.

Main geological features of the modelled area

The polluted aquifer is located in the important groundwater area of Järvelä, in a NW-SE-oriented esker chain in the foreland of the Salpausselkä I marginal formation. Part of the groundwater area is unconfined and part is confined. The bedrock of the area for which the model was constructed is predominantly intact mica gneiss, and a bedrock ridge runs in a north-south direction to the north of the sawmill, separating the esker area proper from a bedrock depression. The flux of groundwater and perched water into this depression is regulated by discharge from the direction of Lake Hähkäjärvi. The depression evidently served as a route by which the chlorinated phenols were transported from the sawmill into the Pyhäoja valley, the permeable soil layers increasing in thickness from half a metre in the area of the sawmill to over 30 m in the valley. The polluted water intake is located in the valley, on the north side of the brook. Groundwater containing chlorinated phenols is moving constantly through the valley and to the north of the Tolkonlähde water intake towards Lake Valkjärvi, and also discharges into the brook Pyhäoja, which flows into the lake.

Concentrations of pollutants

The geology of the area around the sawmill and the nature of the place where the chlorinated phenols were handled suggest that these chemicals could have been entering the groundwater throughout the history of operation of the sawmill. Chlorinated phenol determinations performed on soil and water samples for the purpose of tracing the extent of the pollution revealed only small quantities in the soil of the sawmill area, partly because the soil

there had been changed. Soil concentrations of the active constituent of the Kemtox S10 preservative used nowadays at the sawmill reached a maximum of 16.6 mg kg^{-1}. By contrast, the chlorinated phenol concentrations in the groundwater samples were extremely high, culminating in a figure of almost 100 000 μg l^{-1} in one observation tube in the bedrock depression. A limited comparative survey of the chlorinated phenol determinations nevertheless pointed to considerable discrepancies between the laboratories. The results used here are based mainly on the gas chromatographic methylization and acetylization methods employed by the Research Laboratory of the Water and Environment Research Institute.

Applicability of the MOC model to the Kärkölä case

The suitability of the two-dimensional finite difference solute transport model MOC (Method of Characteristics) used by the Water and Environment Research Institute was tested in the polluted area. The flow equation is approximated by an implicit finite difference equation and the approximation of the transport equation is based on the method of characteristics. The model describes both steady-state and transient changes in the concentration of a non-reactive solute in flowing groundwater. The model assumes that the fluid density, viscosity and temperature gradients do not affect the velocity distribution. The aquifer may be heterogeneous and anisotropic. The groundwater heads or flow rates are used as boundary conditions.

Used correctly, the MOC model is applicable to the small, heterogeneous groundwater area of Järvelä within certain limits. The transport equation is solved by an accurate method of characteristics when only a small amount of numerical dispersion occurs. The modified version used here cannot be said to be user-friendly, however, and it is important that the model should contain efficient input and output programs. The model is well documented, and consequently changes can be made to the code. One drawback is that it requires an even grid of nodes and cells, so that the resolution of one area of interest cannot be improved without increasing the density of the whole grid. In the case of Finland, where abrupt changes in the local

permeability of the surficial deposits are common, it is inconvenient that only one effective porosity value can be inserted into the model. In order for the program to be able to cope with the calculations, the local transmissivity values need to be averaged. The shape and boundaries of the area to be modelled can also lead to inaccuracies, as the grid does not conform exactly to the geological boundaries of the area to be modelled. Also, the fact that the polluted area is confined in places and unconfined in others in the esker area causes variations in the real thicknesses of the saturated highly permeable soil layers.

In addition, the MOC model is able to describe the behaviour of chemical substances only to a limited degree. In cases like the Kärkölä one, for instance, the transport of chlorinated phenols can be depicted only in terms of total concentrations, and it is not possible to examine the fate of the various components of the compound Ky5 separately. The work reported here represents a worst case scenario on relative modelling of the total chlorinated phenol concentrations, as this MOC model application does not take account of any chemical reactions in which they may be involved, nor does it allow the gradients in fluid density, viscosity or temperature to affect the velocity distribution.

Input data and reliability of the calibration

The model was used in order to obtain a better overall understanding of the heterogeneous geology of the area and the sensitivity of the aquifer to environmental changes, and it was tested mainly with research data that had been collected mainly for water supply and supervision purposes in the district of Kärkölä in the period 1970–1990. Information was obtained on the level of the bedrock surface and the degree of bedrock fracturing by means of drillholes extending down to the bedrock and seismic refraction soundings. These field investigations were then filled out with laboratory determinations of grain-size distribution and permeability in order to estimate the thickness of the conductive layer in the area, its hydraulic conductivity and its diffuse recharge. The final hydraulic conductivity values for insertion in the model were then determined by calibration. In addition to the 41 background values, groundwater heads were measured 2–10 times a

year in 18 observation tubes installed in the area. These groundwater heads for the permeable areas were set as boundary conditions for the model, while measurements of the overflow at the springs in the brook Pyhäoja were taken to represent the groundwater discharge from the area. The transport of chlorinated phenols was examined according to the worst-case scenario, in which there are no reactions or adsorption of the chemicals. The remainder of the parameters for the MOC model were estimated on the basis of the geology of the area and information acquired from the literature.

It is the boundary conditions that constitute the most sensitive source of error, for not even precise measurements of hydraulic conductivity can assist in obtaining reliable predictions with the model if erroneous groundwater head data are used as the boundary values. This application of the model is also sensitive to the transmissivity values inserted into it.

Each groundwater area modelled is an individual case, and each requires determination of its own boundary and initial conditions. Thus the groundwater flow result obtained as the solution to a model in each case is unique and cannot be applied to any other area.

The results obtained from applying a model of this kind cannot be any more accurate than the input data. Individual precise measurements, e.g. of hydraulic conductivity properties and groundwater heads, represent only local properties of the aquifer, whereas the values to be assigned to the grid cells are mean aquifer properties applying to the whole area. Thus all applications of the model to the solution of particular problems call for generalizations to be made. In a real groundwater flow system there may well be appreciable differences between the flow rates and directions in different layers and at adjacent observation points, but if the hydraulic conductivity values vary within a small area and in adjacent cells, the program will no longer be able to cope with the calculations. In such cases the higher value of the two hydraulic conductivities for adjacent grid cells in the bedrock depression area, for instance, was used here, thus emphasizing the greater flow rate. The real flow rate is increased relative to that calculated by the model on account of the greater than average influx of perched groundwater into the bedrock depression at times of high runoff. It

would be possible to include variable influx situations of this kind in the MOC model if observations on the groundwater heads were available both over a sufficiently long period and at sufficiently frequent intervals. Trial and error calibration is a flexible approach, but its reliability is greatly dependent on the geological data available.

The mass balance error of water in the flow modelling is less than 0.01 %, and the mean error of mass balance of the chemical is 5 % in transport modelling. Thus the error may be regarded as small and the numerical solution as good. The groundwater heads calculated by the model correspond fairly well to the measured values, and the simulation of the spread of the pollutant is at least indicative of a certain trend. The mean absolute error in the groundwater heads is 0.62 m and the mean error –0.18 m. The results calculated by the model represent average flow and transport situations.

Transport of chlorinated phenols

The calculations suggest that a substantial period of time will be required for the groundwater intake area to be cleaned by natural groundwater flow. If the fire of 1976 is taken as representing a single pollution event, the simulation indicates how far the chlorinated phenols that entered the groundwater on that occasion had travelled in the first 12 years, i.e. by 19.5.1988, the solution being that they occurred over the whole distance of 1.5 km between the pollution site and the outflow area. Simulations also indicate that chlorinated phenols enter the Pyhäoja valley in 6 years after a pollution event.

The fact that there were several instances of the release of .unknown quantities of chlorinated phenols, so that the model cannot be calibrated with respect to their concentrations, means that no accurate comparisons of the transport of these substances can be made between measured and calculated concentration values using this application of the model. Calibration of pollutant concentrations and accurate prediction of their transport has proved possible in corresponding applications if either the times of release or the order of magnitude of the releases have been known. More accurate calibration would have been possible in the present case with respect to the bedrock depression area if accurate

hydrological data had been available for the period preceding the pollution at the Kukonmäki water intake.

Restoration of the polluted area

As there are many factors that affect the transport of contaminants in a heterogeneous groundwater area, groundwater modelling enables more reliable and more illustrative predictions to be made than does monitoring of contaminant concentrations alone. In cases such as that at Kärkölä, the rate and direction of transport of the contaminant and its dilution can be modelled and protective measures can be planned to prevent its spread. The model was used here to simulate the effect of pumping on groundwater heads and water quality, and these results could be applied to the planning of operations to clean polluted groundwater by pumping or protective action.

The calculations suggest that the Kukonmäki water intake is not the best place for pumping out the polluted groundwater, as the large flux towards it from the esker area serves to increase the amounts to be pumped. A better pumping site at the first stage of restoration would be one in the Pyhäoja valley, as the highest concentrations of polluted water flow in this direction. Pumping at the times of high runoff in spring and autumn would then cause an inflow of groundwater to wash the chlorinated phenols out of the layers occupying the bedrock depression, layers in which no groundwater flow exists when the inflow from the Lake Hähkäjärvi direction is at its minimum. At other times of year, when the groundwater flow and groundwater gradient in the depression are below average, pumping from it would be justified, as the heavy concentration of chlorinated phenols there is not washed out by the natural inflow of water.

Reliability of two-dimensional flow and transport modelling for small heterogeneous aquifers

A model is an efficient tool for studying aquifers or situations which cannot be assessed by means of field tests, and is often the best available alternative for analysing a complex groundwater system. Mathematical models provide a better impression of flow and transport velocities than do traditional research methods alone, because a

model cannot make flow calculations if the water balance is not in order. Two-dimensional groundwater modelling is suitable within certain limits for predicting groundwater flow and pollutant transport in the case of a small, heterogeneous aquifer as at Kärkölä, although the heterogeneity of the stratigraphy studied here forces one to make a critical analysis of the results in individual grid cells at the calibration stage. Part of the area concerned here is sensitive to changes in hydraulic regime, and groundwater flow conditions have varied throughout the history of groundwater surveillance in the area, i.e. from the 1970's onwards, and thus a three-dimensional approach is required for detailed analysis, especially in the case of pollutant transport. Two-dimensional vertically averaged descriptions do not capture many of important features needed to predict contaminant movement and cleanup programs. A two-dimensional model nevertheless creates a good framework for expansion of the examination into three dimensions, if only by drawing attention to the points of uncertainty, i.e. the results of the sensitivity analysis can be used when planning further, more detailed modelling studies. A detailed three-dimensional model could be constructed of the area or some part of it, such as the groundwater conditions in the present bedrock depression, if one was familiar with the details of the aquifer and its sensitivity to various hydraulic changes. It is justified in such applications to take account of as many transport factors as possible. The precondition for more detailed modelling of this kind is the existence of more detailed research data than are available at present regarding the geological stratigraphy of the limited area concerned, the occurrence of chlorinated phenols and the question of from which layers polluted water seeps out at the small springs. The choice of a three-dimensional model cannot alone guarantee accurate results if the input data are not three-dimensional. The accurate application of groundwater models, especially three-dimensional ones, requires extensive field data for input and calibration purposes, since the model allows for more efficient use of the available data and can account for more complexities.

A model does not replace fieldwork, but rather the intention is that it should serve as a summary of the results of that work. A model provides a framework for synthesizing field information and for testing ideas on how the system works by means of calibration and sensitivity analyses. Geological factors are nevertheless such that one cannot always obtain all the input data that would be necessary in theory into order to be thoroughly representative of the area concerned. Incorrectly performed pumping tests in a case of groundwater pollution can in fact inflict more damage by altering the directions of flow than it provides new information. In the Kärkölä incident reported on here, polluted pumping water would have constituted a large volume of problem waste of a kind that it is not yet possible to dispose of successfully. Analysis and interpretation of the geological source data is an integral part of groundwater modelling, and missing items can be filled in from the available geological information and by calibration of the model.

Transformation of the data into numerical form takes time, and the modeller needs to know the level of accuracy at which the figures have to be supplied and how much one can or must make generalizations without detracting too markedly from the accuracy of the modelling. An extremely heterogeneous aquifer, for example, should not be rendered too homogeneous by the manner in which the data are fed into the model. A clear qualitative and quantitative conceptual model is required for modelling purposes.

A model that is easy to use may provide a result with little expenditure of effort on the part of the modeller, and without requiring any knowledge of the scientific basis for the work or the reliability of this result. Apart from a knowledge of the large number of reliable methods available for the modelling of pollutant transport, research groups also need to be well versed in hydrology, geology, chemistry, and the models they are using. As practical applications of groundwater models increase in number and diversity, considerable biological and microbiological expertise will be needed for their successful use.

Future needs for the development of groundwater models and input data measurement methods

Rapid progress is being made in groundwater modelling at present, and future models can be expected to make more use of the variances and

correlations attached to hydraulic properties rather than their mean values. New models will also have to be devised to describe complex reactions taking place in the course of pollutant transport.

The adoption of more complex and more accurate models will also call for the development of new field investigation and measurement methods, however. As much geological information as possible should be available for the determination of values of hydraulic conductivity and porosity, in order to calculate more reliable flow velocities. It is difficult to assess the heterogeneity of a groundwater area and its effects are hard to define, and in this sense more attention needs to be paid to field measurement techniques and conceptual models. Concentrations, hydraulic conductivities and effective porosities are properties which should be examined on the same scale, on which all these properties are able to vary within the same area in reality, independent of one another. The uncertainty attached to the real flow velocity and distribution of pollutant concentrations is usually compensated for in practice by means of a dispersion coefficient. The more precisely it is possible to define the flow velocity and concentration, the more accurately the variation in dispersion can be determined and the model calibrated. In general terms, one can say that the parameters in a model that have to be determined by calibration are the more reliable the smaller the number of estimated variables.

Use of models in decision-making

Although application of a groundwater model may be time-consuming and data collection expensive, it is often the best means of making an informed analysis of predictions regarding a groundwater system. Modelling is becoming an increasingly common research and planning tool, enabling the optimization of research resources, technical solutions and groundwater reserves. The use of models in surveys of groundwater areas for water supply purposes could create facilities for rational, rapid investigations of future instances of contamination. Such facilities could also be created in the case of important groundwater areas where these have large accumulations of industry nearby, by appending a calibrated groundwater model to the prospective protection plans drawn up for use in the event of a contamination incident.

YHTEENVETO

Kärkölän kunnassa Järvelän taajamassa sijaitsevalle sahalle asetettiin velvoitetarkkailu, koska sahalla on käytetty puunsuojaukseen Ky5-valmistetta 1930-luvulta vuoteen 1984 asti. Ky5-valmisteen pääkomponentit ovat tri-, tetra- ja pentakloorifenoleita. Sahalta 800 metrin päässä sijaitsevan vedenottamon pilaantuminen havaittiin joulukuussa 1987. Vedenottamon kloorifenolipitoisuudet ylittivät lääkintöhallituksen suositteleman raja-arvon 10 µg l^{-1} noin kymmenkertaisesti ja vedenottamo suljettiin.

Mallinnetun alueen tärkeimmät geologiset ominaisuudet

Kärkölän pilaantunut pohjavesialue sijaitsee ensimmäisen Salpausselän etumaastossa luode-kaakko-suuntaisella harjujaksolla, Järvelän tärkeällä pohjavesialueella. Pohjavesialue on osittain vapaapintainen ja osittain paineellinen. Mallinnettavan alueen kallioperä on pääasiassa ehjää kiillegneissiä. Saha-alueen pohjoispuolella pohjois-etelä-suuntainen kallioselänne on varsinaisen harjualueen ja kalliopainanteen välissä. Hähkäjärven suunnalta virtaavan pohja- ja orsiveden määrä säätelee vedensyöttöä kalliopainanteen pohjavedeksi. Kalliopainanne on toiminut kloorifenolien kulkeutumisreittinä sahalta Pyhäojan laaksoon. Vettäjohtavien maakerrosten paksuudet kasvavat saha-alueen puolesta metristä yli 30 metriin Pyhäojan laaksossa. Pilaantunut vedenottamo sijaitsee Pyhäojan laaksossa Pyhäojan pohjoispuolella. Kloorifenolipitoinen pohjavesi kulkeutuu koko ajan edelleen Pyhäojan laakson kautta Tolkonlähteen vedenottamon pohjoispuolelta länteen Valkjärven suuntaan. Kloorifenolipitoista pohjavettä purkautuu myös Pyhäojaan, joka laskee Valkjärveen.

Lika-aineiden pitoisuudet

Saha-alueen geologian ja kloorifenolien käsittelyalueen sijainnin perusteella kloorifenoleita on voinut päästä pohjaveteen koko sahan käyttöhistorian ajan. Likaantumisen laajuus määritettiin maa- ja vesinäytteistä tehdyillä kloorifenolimäärityksillä. Saha-alueen maanäytteistä löytyi vain pieniä kloorifenolimääriä osittain siksi, että saha-alueella on tehty massan vaihtoja. Nykyisin sahalla käytettävää Kemtox S10 -tehoainetta löytyi maanäytteistä maksimissaan 16,6 mg kg^{-1}. Pohjavedestä löydetyt kloorifenolipitoisuudet sitävastoin ovat erittäin suuria. Suurin havaittu kloorifenolipitoisuus lähes 100 000 µg l^{-1} on määritetty kalliopainanteen alueelta. Suppean kloorifenolimääritysten vertailututkimuksen perusteella eri laboratorioiden kloorifenolimäärityksissä on melkoisia eroja. Tämän tutkimuksen analyysitulokset pohjautuvat pääasiassa vesi- ja ympäristöhallituksen tutkimuslaboratorion käyttämiin kaasukromatografisiin metylointi- sekä asetylointimenetelmiin.

MOC-mallin soveltuvuus Kärkölän likaantuneen akviferin mallinnukseen

Vesi- ja ympäristöhallituksella käytössä olevan MOC-mallin (MOC = Method of Characteristics) soveltuvuutta testattiin pilaantuneen tutkimusalueen pohjaveden virtauksen ja kloorifenolien kulkeutumisen mallintamisessa. MOC-malli on differenssimenetelmään perustuva kaksiulotteinen malli. Malli pystyy kuvaamaan muuttuvaa virtausta sekä aineen sorptiota ja lineaarista hajoamista, mutta sillä ei voi kuvata kemiallisia reaktioita. Nesteen tiheys, viskositeetti ja lämpötila oletetaan vakioiksi. Vettäjohtava kerros voi olla heterogeeninen ja anisotrooppinen. Mallin reunaehdoiksi annetaan pohjavedenkorkeudet tai virtaamat reunoilla.

MOC-malli soveltuu oikein käytettynä monimutkaisen pienen Järvelän pohjavesialueen mallintamiseen. Kulkeutumisyhtälö ratkaistaan tarkalla karakteristika-menetelmällä, jolloin keinotekoista sekoittumista, numeerista dispersiota on vähän. Tässä tutkimuksessa käytetty MOC-mallin versio ei ole käyttäjäystävällinen. Käyttäjäystävällisyyttä tulisi parantaa erityisesti syöttötiedostojen ja tulostuksen osalta. Hyvän dokumentoinnin ansiosta malliin voi tehdä itse muutoksia. Malli vaatii tasavälisen hilapisteverkon, jolloin mielenkiintoisen alueen resoluutioita ei voida tarkentaa tihentämättä koko tutkimusalueen hilaverkkoa. Suomen maaperäoloissa muutokset alueellisessa vedenjohtavuudessa ovat usein jyrkkiä. Malliin voidaan antaa vain yksi tehokkaan huokoisuuden arvo. Vedenjohtokyvyn arvoja on jouduttu paikoitellen keskimääräistämään runsaasti, koska malli ei muuten suoriudu laskennasta. Mallinnettavan alueen muoto ja reunat voivat aiheuttaa epätarkkuutta, koska hilaverkko ei noudata täydellisesti mallinnettavan alueen geologisten

reunojen muotoja. Pilaantunut pohjavesialue on osittain paineellinen ja harjualueella osittain vapaapintainen. Tämä aiheuttaa paksuusvaihteluita todellisissa hyvin vettäjohtavissa pohjavesikerroksissa.

MOC-malli pystyy vain rajoitetusti kuvaamaan kemikaalien käyttäytymistä. Esimerkiksi Kärkölän kaltaisissa tapauksissa kloorifenolien kulkeutumista pystytään käsittelemään vain kokonaispitoisuuksina ja Ky5-liuoksen eri komponenttien tarkastelu ei ole mahdollista. Tässä työssä esitetään pahimman kokonaiskloorifenolipitoisuuden suhteellista mallintamista, koska MOC-malli ei ota huomioon kloorifenolien kemiallisia reaktioita eivätkä gradientit nesteen tiheydessä, viskositeetissa ja lämpötilassa vaikuta virtausnopeuden jakaumaan.

Lähtötiedot ja kalibroinnin luotettavuus

Mallia on käytetty, jotta ymmärrettäisiin paremmin kokonaisuutena tutkimusalueen heterogeeninen geologia ja akviferin herkkyys. MOC-pohjavesimallia testattiin pääasiassa vedenhankinnan ja valvonnan tarpeisiin 1970–1990-luvuilla kertyneellä Kärkölän tutkimusaineistolla. Kallion pinnan tasosta ja kallioperän rikkonaisuudesta saatiin tietoa kallionpintaan ulottuvilla kairauksilla ja seismisillä refraktioluotauksilla. Maastotutkimusten lisäksi laboratoriossa tehtyjen maalaji- ja vedenläpäisevyysmääritysten perusteella arvioitiin tarkasteltavan alueen vettäjohtavan kerroksen paksuus, sen vedenjohtavuus ja imeytymiskerroin. Lopulliset mallille annetut vedenjohtavuusarvot määritettiin kalibroinnilla. Pohjaveden pinnankorkeuden 41 tausta-arvon lisäksi mallialueella on 18 havaintoputkea, joista seurataan vedenpintoja 2–10 kertaa vuodessa. Vettäjohtavilla alueilla pohjaveden pinnankorkeudet asetettiin mallin reunoiksi. Lähteiden ylivirtaaman ja Pyhäojan virtaaman mittauksilla arvioitiin mallialueelta purkautuvia pohjavesimääriä. Kloorifenolien kulkeutuminen on käsitelty pahimpana lika-aineiden kulkeutumistilanteena, jossa kloorifenoleilla ei ole reaktioita eikä pidättymistä. Alueen geologian ja kirjallisuudesta saatujen tietojen perusteella arvioitiin loput MOC-mallille annettavat parametrit.

Reunaehdot ovat herkin virhelähde. Edes tarkat mitatut vedenjohtavuusarvot eivät auta saamaan luotettavia mallinnusennusteita, jos mallin reuna-arvoiksi on annettu virheellisiä vedenpintoja. Mallisovellutus on myös herkkä sille syötetyille vedenjohtavuusarvoille.

Jokainen mallinnettu pohjavesialue on erillinen tutkimuskohde. Pohjavesimalleja käytettäessä jokaiselle tutkimusalueelle pitää määrätä omat reunaehdot ja lähtötiedot. Ratkaistu mallinnettu pohjaveden virtaustilanne ei ole suoraan sovellettavissa toiseen mallinnettavaan alueeseen.

Mallilla laskettujen tulosten tarkkuus ei ole parempi kuin malliin syötettyjen lähtötietojen tarkkuus. Yksittäiset tarkat mittaustiedot esimerkiksi vedenjohtavuusominaisuuksista ja pohjaveden painetasoista edustavat vain paikallisia akviferin ominaisuuksia. Mallin hilaruutuihin annettavat arvot ovat keskimääräisiä akviferin ominaisuuksia koko hilaruudun alueella. Kaikkiin mallisovelluksiin joudutaan sisällyttämään yleistyksiä ongelman ratkaisemiseksi. Todellisessa pohjavesivirtaustilanteessa eri kerroksissa ja hyvin vierekkäisissä havaintopaikoissa virtausnopeudet ja virtaussuunnat voivat erota huomattavasti keskimääräisistä nopeuksista ja suunnista. MOC-malli ei selviydy laskennasta, jos vedenjohtavuusarvot vaihtelevat runsaasti pienellä alueella vierekkäisissä hilaruuduissa. Tällaisissa tapauksissa esimerkiksi kalliopainanteen alueella vedenjohtavuusarvoina on käytetty vierekkäisten hilaruutujen vedenjohtavuusarvoista suurempaa lukuarvoa painottaen nopeampaa virtaustilannetta. Luonnossa todellista virtausnopeutta puolestaan lisää mallin laskemaan nopeuteen verrattuna runsaiden valumien aikana tavallista suuremmat orsiveden purkaumat kalliopainanteen pohjavedeksi. Tällaisten erilaisten vedensyöttötilanteiden kytkeminen MOC-malliin olisi mahdollista, jos käytettävissä olisi sekä riittävän pitkältä seuranta-ajalta että riittävän tiheästi pohjaveden pintahavaintoja. Yritys- ja erehdyskalibrointi on joustava kalibrointitapa. Menetelmän luotettavuus on voimakkaasti riippuvainen saatavilla olevasta geologisesta aineistosta.

Virtausmallinnuksessa massataseen virhe on alle 0,01 prosenttia. Kulkeutumismallintamisessa massataseen virhe on keskimäärin viisi prosenttia. Koska massataseen virhe on pieni, numeerista ratkaisua voidaan pitää hyvänä. Mallilla lasketut ja mitatut vedenpinnat vastaavat melko hyvin toisiaan ja simuloitu lika-aineiden leviäminen on suuntaa-antava. Laskettu pohjaveden painetasojen absoluuttinen virhe on 0,62 m ja keskimääräinen virhe –0,18 m. Mallin laskemat tulokset ovat keskimääräisiä virtaus- ja kulkeutumistilanteita.

Kloorifenolien kulkeutuminen

Mallinnustulosten perusteella kuluu kymmeniä vuosia ennen kuin vedenottamoalue puhdistuu luonnostaan. Laskelmien perusteella kloorifenolien kertapäästön ja 12 vuotta kestävän tasaisen virtaustilanteen jälkeen lika-aineita esiintyy päästökohdan ja mallialueen ulosvirtauskohdan välillä koko 1,5 km matkalla. Jos kertapäästönä pidetään vuonna 1976 tapahtunutta tulipaloa, simulointi havainnollistaa, mihin asti palon aikana pohjaveteen päässeet kloorifenolit ovat kulkeutuneet kahdentoista vuoden kuluttua (19.5.1988). Kuudessa vuodessa lika-aineet kulkeutuvat päästökohdasta Pyhäojan laaksoon.

Tämän tutkimuksen mallisovelluksella ei voida tehdä tarkkoja kloorifenolikonsentraatioiden kulkeutumisvertailuja mitattujen ja laskettujen pitoisuuksien välillä, koska kloorifenolipäästöjä on tapahtunut useina ajankohtina, tuntemattomia määriä ja mallia ei ole siksi pystytty kalibroimaan konsentraatioiden suhteen. Kalliopainanteen alueen lika-ainepitoisuuksien kalibrointi olisi lisäksi täsmentynyt, jos käytössä olisi ollut tarkkoja hydrologisia tietoja Kukonmäen vedenottamon pilaantumisen ilmenemistä edeltävältä ajalta. Vastaavissa mallisovelluksissa lika-ainepitoisuuksien kalibrointi ja tarkat lika-aineiden konsentraatioiden kulkeutumisennusteet ovat mahdollisia, jos tunnetaan joko päästöajankohdat ja päästömäärien suuruusluokka.

Likaantuneen alueen kunnostus

Koska lika-aineiden kulkeutumiseen heterogeenisella pohjavesialueella vaikuttavat monet tekijät, pohjavesimalleilla pystytään antamaan luotettavampia ja havainnollisempia ennusteita kuin pelkillä lika-aineiden pitoisuuksien seurannalla. Kärkölän kaltaisissa tapauksissa voidaan mallintaa lika-aineiden kulkeutumisen nopeutta, suuntaa ja laimenemista sekä suunnitella suojaustoimenpiteitä likaantumisen leviämisen estämiseksi. Tässä tutkimuksessa mallilla on simuloitu vedenoton vaikutusta pohjavedenpintoihin ja laatuun. Näitä tuloksia voidaan soveltaa esimerkiksi suunniteltaessa puhdistuspumppauksia tai suojaustoimenpiteitä.

Laskelmien perusteella Kukonmäen vedenottamo ei ole paras mahdollinen paikka puhdistuspumppauksille, koska vedenottamolle harjualueelta virtaavat suuret pohjavesimäärät lisäävät pumputtavan veden määrää. Pohjaveden puhdistamisen ensimmäisessä vaiheessa puhdistuspumppauspaikka voisi olla Pyhäojan laaksossa, johon virtaavat kloorifenoleilla konsentroituneimmat pohjavedet. Pumputtaessa suurimpien valuntojen ajankohtina syksyllä tai keväällä pohjavesi huuhtelee kloorifenoleita kalliopainanteen kerroksista, joissa ei virtaa pohjavettä Hähkäjärven suunnalta tulevan virtauksen ollessa vähäisimmillään. Pumppaus kalliopainanteesta olisi myös perusteltua vuodenaikoina, jolloin kalliopainanteen pohjavesivirtaus ja pohjavesigradientti ovat keskimääräistä pienempiä ja veden luonnollinen laimeneminen vähäistä.

Pienen heterogeenisen akviferin virtaus- ja kulkeutumismallinnustulosten luotettavuus

Malli on tehokas apuväline tutkittaessa sellaisia akviferin ominaisuuksia tai tilanteita, joita ei voida tutkia kenttäkokein. Mallintaminen on usein paras olemassa oleva menetelmä monimutkaisten pohjavesiolosuhteiden tarkastelussa. Matemaattisilla malleilla saadaan perinteisiä tutkimusmenetelmiä parempi käsitys pohjaveden virtaus- ja kulkeutumisajoista, koska malli ei pysty laskemaan virtausta, jos vesitase ei ole kunnossa. Pohjavesien kaksidimensioinen mallintaminen soveltuu rajoitetusti ennustettaessa pohjaveden virtausta ja lika-aineiden kulkeutumista Kärkölän kaltaisessa pienessä heterogeenisessa akviferissa. Toisaalta tutkittu heterogeeninen stratigrafia pakottaa analysoimaan kaksidimensioisia mallintamistuloksia kriittisesti hilaruuduittain ennen kuin malli on kalibroitu. Osa tutkimusalueesta on herkkä hydraulisissa oloissa tapahtuville muutoksille ja pohjaveden virtaukset ovat vaihdelleet pohjavesitutkimusten tarkkailuhistorian ajan 1970-luvulta lähtien. Kolmedimensioista lähestymistapaa tarvitaan tutkittaessa yksityiskohtaisesti erityisesti lika-aineiden kulkeutumista. Kaksidimensioinen yksikerrosmalli ei kuvaa monia tärkeitä muodostuman piirteitä, joita tarvitaan ennustettaessa lika-aineiden kulkeutumista ja suunniteltaessa puhdistusohjelmia. Kaksidimensioinen mallitarkastelu luo hyvät puitteet kolmedimensioiselle tarkastelulle osoittamalla mallisovelluksen epävarmat kohdat. Herkkyysanalyysiä voidaan käyttää hyväksi suunniteltaessa yksityiskohtaisia mallintamisen jatkotutkimuksia. Tutkimusalueesta tai jostain sen osasta, kuten kalliopainanteen pohjavesioloista, voidaan

koota tarkka kolmedimensioinen malli, kun tunnetaan yksityiskohtaisesti akviferi ja sen herkkyys erilaisille muutoksille. Tällaisessa mallisovelluksessa on perusteltua ottaa huomioon mahdollisimman paljon kulkeutumiseen vaikuttavia tekijöitä. Tarkemman mallintamisen edellytyksenä on nykyistä yksityiskohtaisemmat tutkimustiedot rajatun alueen geologisesta stratigrafiasta, tiedot mistä kerroksista pienet lähteet purkavat pilaantunutta vettä ja tiedot kloorifenolien esiintymisestä. Pelkkä kolmedimensioinen mallin käyttö ei tee mallinnustulosta tarkaksi, jos malliin syötettyjä lähtötietoja ei ole kolmessa dimensiossa. Tarkan erityisesti kolmedimensioisen pohjavesimallintamisen edellytyksenä on runsaat lähtötiedot mallin kalibroinnissa. Toisaalta tarkka malli mahdollistaa monimutkaisten prosessien huomioon ottamisen.

Malli ei korvaa kenttätutkimuksia vaan sen tarkoituksena on tehdä yhteenveto tutkimustuloksista. Mallit tarjoavat menetelmän laajan havaintoaineiston hallitsemiseksi, ja mallin kalibroinnilla sekä herkkyystarkastelulla voidaan testata erilaisia systeemin toimintahypoteeseja. Geologisten tekijöiden takia ei aina voida hankkia kaikkia teoriassa tarvittavia lähtötietoja, jotka edustavat hyvin tutkittavaa aluetta. Väärin toteutetuilla pohjaveden likaantumistapauksien koepumppauksilla voidaan jopa aiheuttaa suhteessa enemmän vahinkoa muuttamalla veden virtaussuuntia, kuin mitä saatu tutkimusinformaatio on. Kärkölän kaltaisissa tapauksissa pumputut kloorifenolipitoiset pohjavedet muodostuvat suureksi määräksi ongelmajätettä, jonka hävittämistä ei ole toistaiseksi pystytty ratkaisemaan. Geologisten lähtötietojen jäsentely ja tulkinta ovat oleellinen osa pohjavesien mallintamista. Puuttuvat lähtötiedot arvioidaan saatavilla olevan geologisen tiedon ja mallin kalibroinnin avulla.

Datan muuttaminen numeeriseen muotoon vie aikaa ja mallintajan on tiedettävä tarkkuus, missä muodossa lähtötiedot annetaan ja kuinka paljon voi tai on pakko tehdä yleistyksiä riittävän mallintamistarkkuuden kärsimättä. Esimerkiksi erittäin heterogeenisestä pohjavesialueesta ei pidä tehdä malliin syötettynä liian homogeenista. Mallintamista varten tarvitaan selkeä kvalitatiivinen ja kvantitatiivinen konseptuaalinen malli.

Helppokäyttöinen malli saattaa antaa pienellä vaivalla mallintamistuloksen, vaikka mallintaja ei tuntisikaan työnsä tieteellisiä perusteita ja tuloksen luotettavuutta. Runsaasti tarjolla olevien luo-

tettavien mallien lisäksi lika-aineiden kulkeutumisen mallintaminen edellyttää työryhmiltä riittävää perehtyneisyyttä hydrologiaan, geologiaan, kemiaan ja käytössä oleviin malleihin. Pohjavesimallien käyttösovellutusten lisääntyessä ja monipuolistuessa tarvitaan jatkossa myös biologian ja mikrobiologian asiantuntemusta.

Pohjavesimallien ja lähtötietojen mittaustekniikan kehittymisen tarpeet

Pohjavesimallintaminen on voimakkaassa kehittymisvaiheessa. Tulevaisuudessa malleissa käytetään hydraulisten ominaisuuksien kuvaamiseksi keskiarvojen lisäksi entistä enemmän varianssia ja korrelaatioita. Malleja pitää kehittää edelleen kuvaamaan monimutkaisia lika-aineiden kulkeutumisessa tapahtuvia reaktioita.

Yhä monimutkaisempien ja tarkempien mallien käyttöönoton edellytyksenä on myös maastotutkimusmenetelmien ja mittaustekniikan kehittyminen. Geologista tietoa pitää käyttää mahdollisimman paljon vedenjohtavuuden ja huokoisuuden määrittämiseksi, jotta saadaan laskettua luotettava virtausnopeus. Pohjavesialueen heterogeenisuutta on vaikea tutkia ja sen vaikutuksia on vaikea määrittää. Kenttämittaustekniikkaan ja konseptuaalisen mallin merkitykseen pitäisi kiinnittää enemmän huomiota. Konsentraatio, hydraulinen johtavuus ja tehokas huokoisuus ovat ominaisuuksia, joita tutkitaan samassa mittakaavassa, jossa todellisuudessa jokainen ominaisuus voi vaihdella toisistaan riippumatta samalla alueella. Mallin kalibroinnissa epävarmuus todellisesta virtausnopeudesta ja lika-aineen konsentraation jakaumasta kompensoidaan käytännössä dispersiokertoimella. Mitä tarkemmin virtausnopeus ja konsentraatio on pystytty määrittämään, sitä tarkemmin voidaan määrittää dispersion vaihtelu ja kalibroida malli. Yleistäen kalibroimalla määritetyt malliparametrit ovat sitä luotettavampia mitä vähemmän on estimoitavia muuttujia.

Pohjavesimallien käyttö päätöksenteon apuvälineenä

Vaikka pohjavesimallien käyttö on aikaavievää ja lähtötietojen kerääminen saattaa olla kallista, mallintaminen on usein paras tapa tehdä ennusteita pohjavesimuodostuman käyttäytymisestä. Mallintaminen yleistyy jatkuvasti tutkimuksen ja suunnittelun apuvälineenä. Tutkimuksilla opti-

moidaan kustannukset, tekniset ratkaisut sekä pohjaveden varastoituminen maaperään. Pohjavesialueiden vedenhankinnan selvityksissä käytetyillä mallisovelluksilla luodaan valmiudet mahdollisesti tulevaisuudessa ilmenevien likaantumistapausten järkevään ja nopeaan selvittämi-

seen. Vedenhankinnan käytössä oleville pohjavesialueille, joilla on runsaasti teollisuutta, tulisi luoda ennakkovalmiudet mahdollisten likaantumistapausten selvittämiseen liittämällä kalibroitu pohjavesimalli suojelusuunnitelmiin.

LIST OF SYMBOLS

Symbol	Unit	
b	m	saturated thickness of the aquifer
C	kg m^{-3}	concentration of the dissolved chemical
C'	kg m^{-3}	concentration of the dissolved chemical in a source or sink fluid
CPs		chlorinated phenols (abbreviation)
D_{ij}	m^2 s^{-1}	coefficient of hydrodynamic dispersion (a second-order tensor)
é	m	thickness of a layer of low permeability
g	m s^{-2}	acceleration of gravity (standard value 9,80665 m s^{-2})
H_s	m	hydraulic head in the source bed, stream, or lake
h	m	aquifer head, or hydraulic head
h_s	m	stream head
K	m s^{-1}	hydraulic conductivity
K'	m s^{-1}	hydraulic conductivity of a layer of low permeability
K_{ij}	m s^{-1}	hydraulic conductivity tensor
K_a	m s^{-1}	vertical hydraulic conductivity of the confining layer, streambed, or lakebed
K_x, K_y, K_z	m s^{-1}	hydraulic conductivity in the directions of the x, y and z axes
k	m^2	permeability of the porous medium, spesific permeability
m	m	thickness of the confining layer, stream bed, or lake bed
PCP		pentachlorophenol (abbreviation)
Q	m s^{-1}	rate of withdrawal (positive sign) or recharge (negative sign)
q	m s^{-1}	flow rate or flow per unit surface area of the contact between the aquifer and stream
S	dimensionless	storage coefficient
S_s	dimensionless	specific storativity coefficient
t	s	time
T_{ij}	m^2 s^{-1}	transmissivity tensor
TCP		trichlorophenol (abbreviation)
TeCP		tetrachlorophenol (abbreviation)
V_i	m s^{-1}	seepage velocity in the direction of x_i
W = W(x,y,t)	m s^{-1}	volume flux per unit area (positive sign for outflow and negative for inflow)
x_i and x_j	m	Cartesian coordinates
$\in$		effective porosity of the aquifer
η	Pa s	viscosity of a fluid
ρ	kg m^{-3}	density of a fluid
φ	m	hydraulic head

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Appendix 1. Description of the input data for the model.

Grid descriptors
        Number of columns   24
        Number of rows   28
        X-distance in metres   42.7
        Y-distance in metres   42.7

Time parameters
        Maximum number of time steps in pumping period   1
        Number of pumping periods   1
        Pumping period in years   12.0

Hydrologic and chemical parameters
        Storage coefficient   0.0
        Effective porosity   0.35
        Longitudinal dispersivity in metres   7
        Ratio of transverse to longitudinal dispersivity   0.50
        Ratio of T_{yy} to T_{xx} 1.0

Execution parameters
        Number of iteration parameters   7
        Convergence criteria in ADIP $1 \cdot 10^{-3}$
        Maximum number of iterations in ADIP   200
        Maximum cell distance per move of particles   0.8
        Maximum number of particles   6 400
        Number of particles per node   9

Program options
        Number of observation wells for hydrograph printout   2
        Number of pumping wells   2
        Number of node identification codes   6

Overflow in Tolkonlähde (m^3 s^{-1})   0.01215

Transmissivity (m^2 s^{-1}) $0.0 - 3.0 \cdot 10^{-2}$

Aquifer thickness (m) $0.0 - 30.0$

Diffuse recharge (−) and discharge (+) (m s^{-1}) $-450 \ldots -150$

Constant head (metres over sea level) $84.0 - 93.02$

Initial concentration in source grid (units)   1 000

Appendix 2. Hydraulic heads in observation tubes.

Hydraulic head (m a.s.l) of groudwater in tube no.

Date	201 +93.59 TH)	202 +90.68	203 +96.60	204 +100.02	205 +97.81	206 +103.75	207 +100.11	208 +100.47	210 +95.07	211 +100.77	212 +100.29	213 +100.83	214 +100.80	217 +101.28	218 +100.56	219 +100.58	220 +87,89	222 +88,84
06.04.88	:	:	:	:	:	+90.82	+89.06	+90.96	:	:	+88.07	:	:	:	:	:	:	:
17.-19.04.88	+88.04	+88.25	+88.10	:	:	+90.67	+97.48	:	+88.07	+90.27	:	+89.62	:	+92.48	:	:	:	:
25.04.88	+88.20	+88.39	+88.34	+90.87	+89.16	+91.00	+97.31	+93.61	+88.16	+90.07	**)	+89.71	+94.47	:	:	:	:	:
20.05.88	:	:	:	:	:	:	+97.16	:	:	:	:	:	:	:	+89.87	+90.13	:	+91.73
06.07.88	+88.05	+88.25	+88.27	+90.92	+89.31	+91.11	+96.96	+93.45	+90.22	+90.47	**)	+89.83	+95.90	+99.03	+89.66	+89.98	***)	+91.64
23.11.88	:	:	:	:	:	:	:	:	:	:	:	:	:	+97.86	:	:	:	:
01.12.88	+88.10	+88.23	+88.25	+90.84	+89.36	+90.90	:	:	+87.99	+90.35	:	:	:	:	:	:	:	:
17.04.89	+88.04	+88.25	+88.10	:	:	+90.67	+93.31	+90.51	+88.07	+90.27	:	+89.78	+91.93	+97.37	:	:	***)	+91.54
20.11.89	:	:	:	:	:	+90.83	:	:	:	:	:	:	:	:	:	:	:	:
18.01.90	:	:	:	:	:	:	+91.41	:	:	:	:	:	:	:	:	:	:	:
30.03.90	+88.17	+88.38	+88.46	+91.02	:	:	:	+93.47	+88.17	+90.30	**)	+89.88	+94.13	+93.23	:	+90.13	***)	+92.14
02.04.90	+88.21	+88.39	+88.40	+90.87	:	+90.97	+92.45	+90.57	+88.20	+90.41	:	+89.91	+95.23	+93.18	:	+90.15	+88.21	**)
17.-24.04.90	+88.19	+88.39	+88.42	:	:	+91.00	:	:	:	+90.39	:	+90.00	:	:	:	+90.14	***)	+91.80
26.04.90	:	:	:	:	:	:	+92.54	:	:	:	:	:	:	:	:	:	:	:
16.05.90	+88.09	+88.31	+88.35	+90.97	:	+91.15	+92.58	+90.72	+88.10	+90.43	**)	+89.91	+91.84	+93.02	:	+90.23	+88.19	+91.63
28.06.90	+88.00	+88.20	+88.25	+90.93	:	+91.07	+92.59	+90.67	+88.00	+90.43	:	+89.84	+90.93	+92.89	:	+90.24	+88.09	+91.57
13.08.90	+87.91	+88.13	+88.16	+90.86	:	+90.99	+92.47	+90.55	+87.91	+90.40	:	+89.76	+90.98	+92.80	:	+90.16	+87.92	:
03.09.90	+87.90	+88.10	+88.13	:	:	+90.95	:	:	+87.88	+90.33	:	:	:	:	:	+90.12	:	+91.50
05.09.90	:	:	:	:	:	+90.95	:	:	:	:	:	:	:	+92.72	:	:	:	:
24.09.90	+87.90	+88.10	+88.13	+90.79	:	+90.95	+92.27	+90.44	+87.88	+90.31	:	+89.68	+90.90	+92.73	:	+90.09	+87.90	+91.52
31.10.90	+87.87	+88.08	+88.10	+90.72	:	+90.85	+92.29	+90.39	+87.85	+90.27	**)	+89.61	+90.90	+92.65	:	+90.06	+87.89	+91.49
5.04.91	+87.90	+88.11	+88.04	+90.62	:	+90.73	+91.77	*)	+87.88	+89.97	**)	+89.33	*)+96.50	+92.83	:	+89.81	***)	+91.34
10.04.91	+87.90	+88.09	:	:	+88.96	:	:	:	+87.89	+89.85	:	:	:	:	:	:	:	+91.28
2.09.91	+87.83	+88.02	:	:	+89.02	:	:	:	+87.81	+90.04	:	:	:	:	:	:	:	+91.35
21.04.92	+88.97	+88.13	:	:	+88.94	:	:	:	+87.95	+89.82	:	:	:	:	:	:	:	+91.21
14.09.92	+87.92	+88.13	:	:	+89.16	:	:	:	+87.89	+90.14	:	:	:	:	:	:	****)	+91.61
20.04.93	+87.94	+88.13	:	:	+89.12	:	:	:	+87.81	+90.07	:	:	:	:	:	:	:	+91.40

TH)	Level of observation tube head
*)	Clogged tube
**)	No water
***)	Overflow
****)	No overflow

Appendix 3. The final water balance and chemical mass balance in the calibrated model.

Cumulative mass balance of water (ft^3)

Recharge and injection	$-2.2533 \cdot 10^{+7}$
Pumpage and evapotranspiration withdrawal	$1.6380 \cdot 10^{+8}$
Cumulative net pumpage	$1.4127 \cdot 10^{+8}$
Water release from storage	0.0000
Leakage into aquifer	$8.7368 \cdot 10^{+8}$
Leakage out of aquifer	$-7.3234 \cdot 10^{+8}$
Cumulative net leakage	$1.4134 \cdot 10^{+8}$
Mass balande residual	70248.0
Error (as per cent)	$7.8386 \cdot 10^{-3}$

Rate mass balance of water (ft^3 s^{-1})

Leakage into aquifer	2.3071
Leakage out of aquifer	-1.9339
Net leakage	$3.7322 \cdot 10^{-1}$
Recharge and injection	$-5.9502 \cdot 10^{-2}$
Pumpage and evapotranspiration withdrawal	$4.3254 \cdot 10^{-1}$
Net withdrawal	$3.7304 \cdot 10^{-1}$

Chemical mass balance

Mass in boundaries	0.0000
Mass out boundaries	$-7.5919 \cdot 10^{+7}$
Mass pumped in	0.0000
Mass pumped out	$-4.6644 \cdot 10^{+2}$
Mass lost by decay	0.0000
Mass adsorbed on solids	0.0000
Initial mass adsorbed	0.0000
Inflow minus outflow	$-7.5920 \cdot 10^{+7}$
Initial mass dissolved	$1.4999 \cdot 10^{+8}$
Present mass dissolved	$8.5940 \cdot 10^{+7}$
Change mass dissolved	$-6.4048 \cdot 10^{+7}$
Change total mass stored	$-6.4048 \cdot 10^{+7}$
Compare residual with net flux and mass accumulation:	
Mass balande residual	$-1.1872 \cdot 10^{+7}$
Error (per cent)	0.0000
Compare initial mass stored with chande in mass stored:	
Error (per cent)	5.2552