Modelling of Transport Processes in Porous Media for Energy Applications

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ABSTRACT

Flows in porous media are encountered in many branches of technology. In these phenomena, a fluid of some sort is flowing through porous matrix of a solid medium. Examples of the fluid are water, air, gas and oil. The solid matrix can be soil, fissured rock, ceramics, filter paper, etc. The flow is in many cases accompanied by transfer of heat or solute within the fluid or between the fluid and the surrounding solid matrix. Chemical reactions or microbiological processes may also be taking place in the system.

In this thesis, a 3-dimensional computer simulation model THETA for the coupled transport of fluid, heat, and solute in porous media has been developed and applied to various problems in the field of energy research. Although also applicable to porous medium applications in general, the version of the model described and used in this work is intended for studying the transport processes in aquifers, which are geological formations containing groundwater.

The model highlights include versatile input and output routines, as well as modularity which, for example, enables an easy adaptation of the model for use as a subroutine in large energy system simulations. Special attention in the model development has been attached to high flow conditions, which may be present in Nordic esker aquifers located close to the ground surface. The simulation model has been written with FORTRAN 77 programming language, enabling a seamless operation both in PC and main frame environments. For PC simulation, a special graphic user interface has been developed.

The model has been used with success in a wide variety of applications, ranging from basic thermal analyses to thermal energy storage system evaluations and nuclear waste disposal simulations. The studies have shown that thermal energy storage is feasible also in Nordic high flow aquifers, although at the cost of lower recovery temperature level, usually necessitating the use of heat pumps. In the nuclear waste studies, it was found that the heat generation of the spent fuel has a marked effect on the groundwater flow near the repository for thousands of years, increasing the flow rate at most to five-fold compared to the natural situation.

In the applications, the model has proven to be a versatile tool and easily applicable in various situations. As a future development, the inclusion of unsaturated zone simulation as well as improvements in solute transport routines are being considered.
PREFACE

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1 INTRODUCTION

1.1 Background

Flows in porous media are encountered in many branches of technology. In these phenomena, a fluid of some sort is flowing through porous matrix of a solid medium. Examples of fluid are water, air, gas and oil. The solid matrix can be soil, fissured rock, ceramics, filter paper, etc. The flow is in many cases accompanied by transfer of heat or solute with the fluid or between the fluid and the matrix. Chemical reactions or microbiological processes may also be taking place in the system.

The energy-related applications of porous media range from oil reservoir engineering to thermal energy storage. In oil reservoir engineering, porous medium processes are important both in the forming and in the utilization of the oil reserves. The flow processes are very complicated, involving simultaneous flow of oil, gas and water. The energy storage applications include, most importantly, storage of heat in geologic formations, e.g. in groundwater reservoirs. Porous medium processes are present also in phase change heat storage systems. Although the results obtained here are applicable to porous medium studies in general, the main interest in this thesis was in heat storage in underground formations containing groundwater.

Aquifers, which are geological formations containing groundwater, offer a simple and potential way of storing heat for long periods of time. Long term heat storage is an important issue especially in cold climates, where heat storage can be used to reduce the different time dependence of energy production and consumption. The need for a storage is pronounced with renewable energy sources, such as solar energy. Also, large cogeneration systems benefit from heat storage. Groundwater can also be used directly as a heat source for a heat pump.

Aquifer storage is not a new concept. Since the 1950's aquifers have been used to store fresh water, oil products, natural gas, and liquid wastes (Tsang et al., 1980). Their use for thermal energy storage, however, was not suggested until in the 1970's. A great deal of the work done on aquifer thermal energy storage (ATES) has been reported in international conferences arranged by the International Council on Thermal Energy Storage (ICTES), most recent ones in France (Ferrandes and Despois, 1988), in the Netherlands (Snijders and van Mourik, 1991) and in Finland (Kangas and Lund, 1994). An important forum for international co-operation has been provided by the International Energy Agency's (IEA) implementing agreement on Energy Conservation Through Energy Storage Programme.
Through their intimate link with the environment, aquifers have also an indirect connection with energy systems in general. The pollution released from energy systems may be conducted to groundwater, thus possibly spreading to wide areas. Often, the pollutant is some sort of chemical species released into the ground as a result of accident or leak. The release may also consist of thermal pollution in the form of heated or cooled water, which can lead to unwanted changes in groundwater quality as a result of chemical or biological effects induced by the temperature changes.

Groundwater also forms an important issue in the disposal of wastes resulting from the use of nuclear energy. Much effort is currently focused on the disposal of wastes deep beneath the ground surface in geological formations such as salt mines or bedrock. In case of leakage, transport with groundwater flow provides the most important way for radionuclides to migrate to the biosphere. Groundwater flow may also enhance heat transfer in the vicinity of the disposal site, causing changes in the temperature distribution and in the flow patterns around the repository.

1.2 The aim of the thesis

In the design of aquifer energy storage as well as in the study of groundwater related environmental problems, the ability to evaluate transport processes (fluid, heat, solute) is essential. The need for proper evaluation is emphasized by the large spatial and temporal extent of the problem. By groundwater flow, heat and solutes can be transported to very wide areas. The time constants involved are also usually large. This is reflected, for example, in the fact that the cleaning of a polluted ground may take years. The remediation of groundwater is also a very costly process, which emphasizes the importance of proper design of the cleaning procedures.

Analytical methods can be used in approximate calculations or in some very simplified cases, but in general the analysis of a combined fluid, heat and solute transport is a complicated task in which numerical methods are needed. High groundwater flow rates (several hundreds of meters per year) which can be present in aquifers close to the ground surface in Nordic conditions, still complicate the analysis: the aquifer flow field must be accurately determined in order to be able to predict the movement and range of thermal effects or the spreading of pollutants.

Simulation models for groundwater transport with varying accuracy and complexity have been developed since the 1970's (Tsang et al., 1980). They
range from simplified system models (Mazzarella, 1991) to more refined storage models (Doughty et al., 1982; Hellström et al., 1986) and complex multiphase models for super computer environment (Pruess, 1987).

The purpose of this thesis has been to develop a versatile simulation tool that can be applied to various energy-related applications with the stress, however, being on aquifer energy storage applications. The use of commercial general-purpose program packages such as PHOENICS was excluded because of the desire to gain a deep understanding of the physical processes involved, which is better obtained by developing the code by oneself. Also, the general nature of the commercial packages easily limits the usability and the potential for development of the model.

The factors emphasized in the model development were

- 3-dimensional modelling
- coupling of fluid flow with heat and solute transport
- high fluid flow rates
- energy system analysis
- versatile input and output routines
- spatially varying material properties
- PC environment

A 3-dimensional approach is important in the accurate evaluation of thermal effects, especially buoyancy, as well as in accounting for the coupling between the various transport processes. High fluid flow rate, from tens to few hundreds of meters per year, was considered to be of special importance, as high flows often characterize the so called esker aquifers (Airaksinen, 1978; Iihola et al., 1987), which form an important part of Nordic groundwater resources. These aquifers are located near the ground surface; deeper in the ground the groundwater flow rate is significantly smaller.

Most of the studies so far have concentrated on low flow aquifers (Tsang et al., 1980; Ferrandes and Despois, 1988; Snijders and van Mourik, 1991; Kangas and Lund, 1994). The inclusion of higher flow rates complicates e.g. heat transfer calculations by increasing the relative importance of convection which, especially with 3-dimensional approach, leads to difficulties in calculations, mostly in the form of computational instabilities.
The range of validity of the porous medium approach in heat transfer calculations had also not been thoroughly accounted for previously, and was therefore given special attention in this thesis in a form of a separate study.

The resulting simulation model, THETA, employs the explicit finite difference method (FDM) to discretize the flow equations. FDM was preferred to finite element method (FEM) mostly because of its straightforward applicability and efficiency: most of the published FEM methods employ a direct solution leading to large systems of equations, the solution of which is time consuming (Patankar, 1980). As the main application platform is a microcomputer with less computational power, this was not desired.

The 3-dimensional approach of the model is mirrored in the ability of the model to accept an accurate description of the simulated medium with spatially varying properties. Although the main emphasis in the model development and utilization has been on groundwater analysis, the model is applicable also to more general porous medium problems.

The ability to use THETA on PC also enhances its value as a design tool, microcomputer environment being cheaper and more easily accessible than big main frame computers. A special enhancement of the model is a graphic interface that has been developed for microcomputer environment. The interface enables interactive input data definition as well as on-line visualization of simulation results by showing the advance of simulation in both graphic and numerical form. Excluding the graphics, the model can also be compiled and run in a main frame computer or work station environment.

The model performance has been verified and the thermal part also validated with applications representing a wide range of hydrogeological and system properties. In this thesis, some applications have been included to demonstrate the capabilities of the model.

This thesis consists of a summary and eight publications, as listed below. Publication I is the main model document containing a detailed description of the simulation model. In publication II, a more concise and up-to-date description of the model is given, while publication III includes a description of the model validation. Two thermal energy applications of the model are described in publications IV and V, which give an account of studies on thermal energy storage systems and on heat pumps employing the ground as a heat source, respectively. The simulation studies in publications VI and VII are related to thermohydraulic investigations on nuclear waste disposal. Finally, publication
VIII gives a short description of the solute transport routines and their application.

The author has actively participated in all work reported in the thesis. He has written all the attached publications and performed all the simulations except the SPEOS and packed bed simulations. The simulation program THETA is exclusively coded and written by the author.
1.3 Publications


2 MATHEMATICAL MODEL

2.1 Groundwater and aquifers

The term groundwater in its most general meaning denotes all waters found beneath the surface of the ground. In groundwater studies, however, the term is usually taken to denote the water in the zone of saturation where all ground pores are filled with water. A typical distribution of subsurface water showing the different layers or zones can be seen in Fig. 2.1. The division into different layers is based on the proportion of pore space occupied by water as well as the type of bonding between water and the surrounding ground.

Aquifer is a geologic formation that contains water and permits significant amounts of water to move through it. A confined aquifer is bounded from above and below by impermeable formations. In a phreatic aquifer, the water table itself serves as the upper boundary. If water can penetrate in small amounts through bounding formations, the aquifer is called leaky.

Groundwater forms a part of the natural water cycle, representing one per cent of the total water masses, or about 15 million km$^3$ globally. Water from precipitation infiltrates the ground surface, moves downward, and finally accumulates on some impervious stratum (e.g. bedrock). The groundwater movement mostly takes place in the zone of saturation. Water then moves on, until it finally discharges into a river or sea. The flow rate in porous medium is determined by permeability of the ground, which in turn depends on the amount and structure of the void space in ground. The natural flow rate of groundwater can vary widely, ranging from almost stagnant water up to specific discharge values (m$^3$/m$^2$ cross sectional area) of several hundred meters per year.

Fig. 2.1: Subsurface water (Bear, 1972).
2.2 Porous medium approximation

The flow of fluid through porous medium is a very complicated process, taking place through a complex network of interconnected pores or openings. In practice, it is impossible to trace the movement of fluid at microscopic level inside the individual pores. Instead, a macroscopic description is invoked, in which the flow is described as taking place as a fictitious average flow through the porous medium.

The pores in porous media form the channels through which the fluid flows. The volumetric flow describes the amount of fluid flowing through the porous medium. It is defined as volume of fluid flowing through a cross sectional area per time. Because the flow can only take place through pores, we have for the volumetric flow through a cross sectional pore area $\Delta A_j$:

$$Q_{j0} = \int_{\Delta A_j} v_j \, dA_j \quad ,$$

(2-1)

where $v_j$ is the fluid flow velocity component in the direction $\vec{j}$. The flow rate in porous media is usually described by specific discharge $q$, often denoted simply as flow rate or Darcy flow, the component of which in the direction $\vec{j}$ is defined as the volumetric flow rate ($Q_{j0}$) through the total cross sectional area $(\Delta A_j)_0$:

$$q_{j0} = \frac{Q_{j0}}{(\Delta A_j)_0} \quad .$$

(2-2)

The flow rate $q$, also called specific discharge or Darcy flow, thus actually describes volumetric flow, although it has the dimensions of velocity (m/s). The actual fluid velocity $v$ (c.f. Eq.(2-1)) is

$$\bar{v} = \frac{\bar{q}}{n} \quad ,$$

(2-3)

where $n$ is the effective porosity, defined as a fraction of total pore volume that is available for fluid flow (Bear, 1972).

2.3 Fluid flow

Fluid flow through porous media can be described mathematically by the so called Darcy equation, originating from the experimental work of a French
physicist, Henry Darcy. According to it, the specific discharge is given by (Bear, 1972):

$$q = KJ$$

where $\Phi$ is the piezometric head and $J$ is the hydraulic gradient. For instance in the case of two-dimensional groundwater flow, $J$ describes the slope of the water table. The factor of proportionality, $K$, is called hydraulic conductivity. It is in general a tensor quantity ($\bar{K}$), depending on the properties of both the solid matrix and the flowing fluid.

For more detailed 3-dimensional calculations including also buoyancy flows generated by temperature differences, a more appropriate form of the Darcy equation is:

$$q = \frac{k}{\mu} (\nabla p - \rho g)$$

where $p$ is the pressure, $\rho$ and $\mu$ the fluid density and dynamic viscosity, respectively, and $g$ the acceleration of gravity. The factor of proportionality, $k$, is called the intrinsic permeability, or simply permeability, and it describes the ability of the porous medium to conduct fluid through it. In contrast to water conductivity, the intrinsic permeability is a parameter depending only on the properties of the solid matrix. It is related to $K$ by (Bear, 1972):

$$\bar{K} = \frac{k \rho g}{\mu}$$

Like hydraulic conductivity, the permeability is in general a symmetric tensor quantity, having in three dimensions 6 distinct components which can vary both spatially (heterogeneity) and directionally (anisotropy). Further, by choosing the co-ordinate axis to coincide with the principal directions of anisotropy of the medium, the permeability matrix can be reduced to a form with only three (diagonal) components (Bear, 1972):

$$\bar{k} = \begin{pmatrix} k_{xx} & 0 & 0 \\ 0 & k_{yy} & 0 \\ 0 & 0 & k_{zz} \end{pmatrix}$$
The equation of motion for groundwater is obtained by combining the Darcy equation with the equation of continuity. Confining to non-deformable media and assuming the changes in density to be slow, we can restrict ourselves to equilibrium where:

$$\nabla \cdot (\rho \vec{q}) = Q \quad .$$  \hspace{1cm} (2-7)

Confining further to incompressible flow we get the equation:

$$\nabla \cdot \vec{q} = \frac{Q}{\rho} \quad .$$  \hspace{1cm} (2-8)

which combined with the Darcy equation gives the equation for fluid motion.

The Darcy equation is not universally valid, but has upper and lower limits of applicability. It has been found (Bear, 1972) that the Darcy approximation is valid for the laminar flow regime, where the viscous forces are predominant as compared to inertial forces. Mathematically, this can be stated by requiring that for the porous medium approximation (Darcy law) for flow to be correct, we must have

$$Re \leq 1\cdots10 \quad , \quad Re \equiv \frac{qpd}{\mu} \quad ,$$  \hspace{1cm} (2-9)

where $Re$ is the Reynolds number and $d$ is the mean grain diameter.

With groundwater flow, the limitation (2-9) is usually of no concern. In a typical high flow aquifer consisting of gravel (medium diameter of about 10 mm), for instance, the natural flow rate is about 100 metres/year, giving $Re \approx 0.024$ , which is clearly below the limit. With a natural flow of 1 km/year, we are approaching the limit, especially because larger grain diameters are often associated with a higher groundwater flow rates. One must note, however, that the Darcy equation does not break suddenly, giving instead values differing from the correct ones more and more as the limit is exceeded.

There are indications that there also exists a lower limit for the Darcy approximation in the form of minimum initial gradient $J_0$, below which there is very little flow. The reason for this behaviour is not clear. Non-Newtonian behaviour and small countercurrents are few of the proposed explanations. This phenomenon is not, however, of significance with groundwater flows of practical interest (Bear, 1972).
2.4 Heat transport

Heat is transferred in porous media basically by two processes, conduction and convection. Heat conduction is driven by temperature differences, with no movement of the transferring medium, whereas in convection the medium itself moves. The convection can be either forced or natural, depending on whether it is driven by external forces or temperature differences (buoyancy). Heat conduction takes place also in dry ground with no groundwater present.

In aquifer heat transfer, an equilibrium assumption is usually invoked, stating that groundwater and the surrounding ground are in thermal equilibrium, i.e. they are locally at the same temperature. Heat transfer can then be described by a single equation for the fluid saturated medium. The governing equation for heat transfer can be deduced from the principle of conservation of energy, and it is (incompressible fluid):

\[
\frac{\partial T}{\partial t} + \nabla \cdot (\lambda_s \nabla T) - (\rho c)_f \vec{q} \cdot \nabla T + H = 0,
\]

where \((\rho c)_s\) and \((\rho c)_f\) are the heat capacities per unit volume of the fluid saturated soil and the fluid itself, respectively, \(T\) is the temperature, \(\lambda_s\) the thermal conductivity of the saturated soil, and \(H\) a term representing a heat source or a sink. The first and second terms on the right-hand side of the equation (2-10) give the contribution of heat conduction and convection, respectively.

The appearance of Darcy flow \(q\) instead of actual velocity \(v\) in the convection term is due to the fact that in porous media, only a part of the cross section is available for flow, the rest being filled by the solid matrix. The convective component in the heat balance equation leading to Eq.(2-10) is then in accordance to Eq.(2-3) (x-component):

\[
\dot{Q}_{\text{conv,x}} = (\rho c)_f n v \Delta y \Delta z (T - T_{\text{ref}}) = (\rho c)_f q \Delta y \Delta z (T - T_{\text{ref}}),
\]

where \(\dot{Q}\) denotes change in heat content, \(\Delta z \Delta y\) is the area of volume element perpendicular to the flow, and \(T_{\text{ref}}\) is some reference temperature.

The thermal properties of the water saturated soil (subscript \(s\)) are weighted averages of the appropriate values for water and dry ground, i.e. for volumetric heat capacity we have:
\[(\rho c)_{s} = (1 - n)(\rho c)_{g} + n(\rho c)_{f}, \quad (2-12)\]

where \(n\) is the porosity and the subscripts \(g\) and \(f\) refer to dry ground and water, respectively.

### 2.5 Solute transport

To facilitate the simulation of solute transport in THETA, retardation-based solute transport routines including radioactive decay have been included in the model. With the following assumptions

- only equilibrium-controlled ion exchange reactions and radioactive decay are considered
- adsorption isotherm can be described with a linear and reversible equation \(\overline{C} = K_{d}C\), where \(\overline{C}\) is the concentration of species adsorbed to the solid and \(K_{d}\) is called distribution coefficient.
- the daughter nuclides in the radioactive decay chain are not considered
- dispersion factor (constant) consists of the contribution of molecular and mechanical dispersion.
- water density and viscosity are functions of temperature only (low concentration flows).
- reactions between different species are excluded.

the solute transport equation for incompressible flow takes the form (Javandel et al., 1984):

\[R \frac{\partial C}{\partial t} = D \nabla^{2}C - \vec{v} \cdot \nabla C - \lambda_{d} CR + S, \quad (2-13)\]

where \(C\) is the concentration of solute, \(D\) the dispersion coefficient, \(\vec{v}\) the actual flow velocity, \(S\) a source term, \(\lambda_{d}\) is the radioactive decay constant and \(R\) is a retardation coefficient defined by

\[R \equiv \left(1 + \frac{\rho_{b}K_{d}}{n}\right), \quad (2-14)\]

where \(\rho_{b}\) is the bulk density.

As the main emphasis in this thesis was in the thermal behaviour of the porous media, which are of greater importance in energy-related applications, the transport model is not intended to be comprehensive and it contains many
limitations (c.f. above). However, it can be used in connection of the thermal simulation to give insight into the combined effect of heat and solute transport.

2.6 Validity of the temperature equilibrium assumption

2.6.1 Fourier number analysis

An essential assumption in the derivation of the heat transfer equation is the temperature equilibrium between the solid and fluid phase. This assumption is justified as long as the rate of convective flow is small compared to the time it takes for the solid particles to heat up to the temperature of the fluid surrounding it.

The validity of this assumption can be studied with the help of dimensionless Fourier number, which can be interpreted as the ratio of heat conduction rate to the rate of thermal energy storage in a solid (Incropera and de Witt, 1985). It is also called dimensionless time. For porous media it can be written as:

\[ \text{Fo} = \frac{\lambda_s t}{(\rho c)_s d^2} \]  

(2-15)

where the solid phase grain diameter \( d \) has been used for typical length. With typical high flow groundwater parameters for granite as forming solid phase particles (Iihola et al., 1987):

\[ \lambda_s = 3.5 \text{ W/mK} \] \[ (\rho c)_s = 2.16 \cdot 10^6 \text{ J/m}^3\text{K} \] \[ n = 0.35 \]

we get for particles with a diameter 0.01 m (gravel):

\[ \text{Fo} \approx 0.0162 \frac{1}{s} t \Rightarrow t_{ch} = 62 \text{ s} \]

where \( t_{ch} \) is a characteristic time, for which \( \text{Fo} = 1 \). With groundwater flowing at a rate \( q = 100 \text{ m/y} \), or \( (n = 0.35) v \approx 285 \text{ m/y} \), it advances during the characteristic time a distance of about \( 5.6 \cdot 10^{-4} \text{ m} \), or 5% of the particle diameter. In these circumstances it is thus reasonable to assume that there is no temperature difference between the fluid and the solid.

With flow rate \( q = 1000 \text{ m/y} \), however, the distance covered is already about 50% of the grain diameter and it seems that we are approaching the limit of the
equilibrium assumption. This is the same limit at which the Darcy approximation was above found to be approaching its limits.

### 2.6.2 Packed bed analogy

The validity of the equilibrium assumption was also studied by utilizing the analogy between porous media and a packed bed. Two models, with and without temperature equilibrium assumption, were constructed.

In general, a packed bed is a porous medium, which may consist of plates, cobbles or bricks, between which the fluid flows. From thermal point of view, the main advantage of a packed bed is an increase in the contact area between the solid and fluid, which increases the rate of heat transfer.

Heat is transported both in the solid matrix and in the void system containing the flowing fluid. In the solid matrix, heat is transferred by conduction through the grains and from one grain to another. In the fluid heat is transferred both by conduction and convection.

When hot water and grains differ in temperature, heat will be exchanged between water and solid. By restricting ourselves to a two-dimensional case with flow only in the x-direction, the basic equations describing heat transfer in a packed bed are:

\[
n(\rho c)_f \frac{\partial T_f}{\partial t} + n(\rho c)_f v_x \frac{\partial T_f}{\partial x} = n\lambda_f \frac{\partial^2 T_f}{\partial y^2} + n\lambda_f \frac{\partial^2 T_f}{\partial x^2} + h_v (T_g - T_f)
\]

(2-16)

\[
(1-n)(\rho c)_g \frac{\partial T_g}{\partial t} = (1-n)\lambda_g \frac{\partial^2 T_g}{\partial y^2} + (1-n)\lambda_g \frac{\partial^2 T_g}{\partial x^2} + h_v (T_f - T_g)
\]

(2-17)

where subscripts \(f\) and \(g\) refer to the flowing fluid and solid matrix, respectively, and \(h_v\) is the volumetric heat transfer coefficient, describing the exchange of heat between the solid and the fluid. In low Reynolds-number regime, heat transfer in multiparticle systems can be described by a relation derived from the analysis done by Pfeffer (1964):

\[
\frac{hd}{\lambda_f} = 1.26 \left( \frac{1 - (1-n)^{\frac{1}{2}}}{W} \right) \left( \frac{\rho_f v_f d_f}{\lambda_f} \right)^{\frac{1}{2}}
\]

(2-18)
where subscript \( f \) refers to the fluid, \( d \) is the particle diameter, \( n \) is the porosity, \( v \) the kinematic viscosity and

\[
W = 2 - 3\gamma + 5\gamma^2 - 2\gamma^6, \quad \gamma = \sqrt{1 - n}.
\]  

(2-19)

The surface heat transfer coefficient \( h \) is related to the volumetric heat transfer coefficient used in Eqs. (2-16) and (2-17) by (Schmidt and Willmott, 1981):

\[
h_x A_{cr} = \frac{h A}{L},
\]

(2-20)

where \( A_{cr} \) is the frontal cross sectional area of the packed bed, \( L \) its length and \( A \) the heat transfer surface. By assuming the bed to consist of spherical particles Eq.(2-20) yields

\[
h_x = (1 - n)\frac{6}{d} h.
\]

(2-21)

With temperature equilibrium assumption, we have \( T_f = T_g = T \) and Eqs. (2-17) and (2-18) reduce to (with subscript \( s \) denoting the fluid saturated solid matrix):

\[
\left(\rho c_s\right) \frac{\partial T}{\partial t} + n(\rho c)_f v_x \frac{\partial T}{\partial x} = \lambda_s \frac{\partial^2 T}{\partial x^2} + \lambda_s \frac{\partial^2 T}{\partial y^2}.
\]

(2-22)

On the basis of Eqs (2-16) - (2-22), two simulation models were constructed. The scheme of the two-dimensional packed bed used in the equations is shown in Fig. 2.2. The packed bed, with length \( L \) and width \( W \), consists of pebbles with a uniform diameter. Water enters the packed bed at the front side through a small

![Fig. 2.2: The scheme of the packed bed model.](image)
opening representing a source (temperature $T_{in,hot}$) and leaves it at the rear side ($T_{out}$). Initially, both water and pebbles in the bed are at the same temperature ($T_{in,0}$).

The thermal behaviour of the packed was analyzed by studying the water temperature values near the end of the packed bed. The general form of the breakthrough curves thus obtained is shown in Fig. 2.3 (Felders, 1991). With constant temperature input, the temperature at the far end first remains constant, then starts to rise as the warm water breaks through, and finally levels at a steady state temperature, which is the same for both equilibrium and non-equilibrium models.

The differences of the two approaches can be seen on the rising part of the curve. With the non-equilibrium equations, the water temperature starts to increase earlier, as the water breaks through, leaving the pebbles in slightly lower temperature. At the later part of the curve, the order of the curves is reversed, as the pebbles in the non-equilibrium model cool down the water.

In the simulations, the difference between the two approximations was described by the resulting maximum temperature difference $\Delta T_{max}$ on the breakthrough curve:

$$\Delta T_{max} = \max \left( T_{eq} - T_{non-eq} \right)$$

(2-23)

where the subscripts $eq$ and $non-eq$ refer to the equilibrium and non-equilibrium assumptions, respectively.

The simulations (Felders, 1991) showed that in typical high-flow groundwater
conditions, the temperature differences between the two approaches are generally very small. Figure 2.4 shows one specific example. The ground was assumed to consist of gravel (porosity 40%), and the input temperature was 70°C. The distance of the temperature measurement was 15 m from the input.

As can be seen, with flow velocity of 2 km/year (corresponding to specific discharge \( q = 2 \times 0.4 = 0.8 \text{ km/year} \)), which is already a high value and at the upper limit of Darcy approximation, the maximum temperature difference is only about 0.5°C even with unreasonably high pebble diameter of 10 cm. With more reasonable pebble diameters (e.g., 1 cm for gravel) the difference is very small.

2.7 Boundary conditions

The boundary conditions for water flow and heat or solute transport equations can be either of Neumann or Dirichlet type. In Neumann conditions, typically the normal component of water flow (\( \bar{q} \)), heat conduction (\( \bar{q}_h \)) or solute diffusion (\( \bar{q}_s \)) at the boundary \( \Gamma \) is fixed. The Dirichlet conditions, on the other hand, determine the actual function values at the boundary.

In simulations, one usually chooses the boundaries to be so far that they can be considered undisturbed (Dirichlet conditions). However, if water or heat flow at some boundary is predetermined, boundary conditions of Neumann type must be used.

2.8 Constitutive equations for aquifers

The material parameters in the equations above depend in general on pressure, temperature and concentration. With the assumption of incompressibility implicit
in the equations, the dependence on pressure needs not to be accounted for. Limiting to low-concentration flows, the dependence on solute concentration is also neglected here.

Considering water as the flowing fluid, the changes with temperature in thermal conductivity and heat capacity are here assumed to be relatively small and are neglected. Water density and viscosity cannot, however, be assumed to be temperature independent. To a good approximation, the temperature dependence of the density can be described by

\[ \rho = \rho_0 (1 - \alpha (T - T_0)) , \]  

(2-24)

where \( \alpha \) is a constant and \( \rho_0 \) water density at a reference temperature \( T_0 \). In reality, the dependency of the density on the temperature is not linear, so the coefficients in Eq. (2-24) must be chosen according to the temperature area of interest. For instance, in the temperature domain \( 5^\circ C < T < 75^\circ C \), which was appropriate in the simulation of the Rajamäki hot water injection experiment that was used in the validation of the model (chapter 6.2 and Publication III), using the parameters:

\[ T_0 = 20^\circ C \quad , \quad \rho_0 = 998.2 \, \frac{kg}{m^3} \quad , \quad \alpha = 0.0004 \]

in Eq.(2-24) gives temperature values differing at most 0.4 \% from the tabulated (measured) values.

Viscosity, on the other hand, is in the present version of the model approximated by formulas (Weast, 1975):

\[ 0^\circ C < T \leq 20^\circ C \]

\[ \log_{10} \mu_T = \frac{1301}{998.333 + 8.1855(T - 20) + 0.00585(T - 20)^2} - 1.30233 \] ,  

(2-25)

\[ 20^\circ C < T < 100^\circ C \]

\[ \log_{10} \frac{\mu_T}{\mu_{20}} = \left( \frac{1.3272(20 - T) - 0.001053(T - 20)^2}{T + 105} \right) , \]  

(2-26)

which give \( \mu_T \) in units cp \( (1 \, cp = 10^{-3} \, Ns/m^2) \).
The heat capacity as well thermal conductivity of the fluid saturated matrix (ground in case of aquifers) are calculated as weighted averages of the corresponding values for the dry matrix and the fluid:

\[
\begin{align*}
(\rho c)_s &= n(\rho c)_f + (1 - n)(\rho c)_g , \\
\lambda_s &= n\lambda_f + (1 - n)\lambda_g .
\end{align*}
\] (2-27) (2-28)

where, in case of aquifers, the subscripts \( f \) and \( g \) refer to water and the dry ground, respectively.
3. NUMERICAL MODEL

3.1 Discretization methods

The numerical solution of equations is based on discretization, where the continuous space variables are replaced by their values at discrete locations and by writing the governing equations in terms of these variables. Also, the time is treated as discrete time intervals. The two main methods for discretization are the finite element method (FEM) and the finite difference method (FDM). The FDM is further divided to implicit and explicit methods (Patankar, 1980).

The main advantages of FEM are its ability to accurately reflect complex geometries as well as its stability. The systematic nature of grid generation enables one to device algorithms for automatic grid generation. As to stability, however, the convection in fluid flow simulation can cause problems (Patankar, 1980).

In this thesis, however, the explicit finite difference method was chosen for discretization. The main advantages of the explicit FDM compared to implicit methods are:

- computation speed
- smaller memory requirement
- straightforward applicability

The speed of calculation as well as smaller memory requirement are a result of the explicit nature of the FDM. Implicit methods (like FEM) lead to large systems of simultaneous equations, the solving of which is time consuming, requires a lot of computer memory and usually necessitates the use of complicated algorithms. The smaller need of computer resources is especially important as the model developed here was mainly intended to be used in a microcomputer environment.

The most restrictive disadvantage of FDM is its instability, which limits the size of time step that can be used with a specified spatial accuracy (grid point distance). This was not, however, considered to be a severe limitation, as the intended use of the model was in the study of heat storage dynamics, which in itself requires small time steps.

3.2 Finite difference method

The numerical approach is described in detail in Publication I. Here, only the most relevant features of the solution are described.
In FDM, the variables in the equations are approximated by their values at discrete grid points. For the derivatives, describing the change or rate of change of the variables, different approximations can be used. Most often, the so called central or forward/backward differences are used (Patankar, 1980; Lunardini 1981). Central difference is second order accurate ($\Delta x^2$), whereas forward and backward differences are first order accurate ($\Delta x$).

In the model presented in this thesis, central differences were used for conduction/dispersion terms. In the convective parts of the equation, however, stability problems necessitated the use of the so called upwind method, which employs forward and backward differences. In this method, e.g. the convective heat transport term in x-direction is approximated as:

$$\left(q \cdot \nabla T\right)_x \approx \left(\frac{T_{i,j,k} - T_{i-1,j,k}}{\Delta x}\right) \max(q_x,0) + \left(\frac{T_{i+1,j,k} - T_{i,j,k}}{\Delta x}\right) \min(q_x,0), \quad (3-1)$$

where $q_x$ is the $x$-component of the specific discharge, $T$ is the temperature and the abbreviation max (min) means the maximum (minimum) of the values in the parenthesis. The flow direction is assumed to be positive in the direction of increasing $i$-index. Thus, in this approximation, the temperature gradient is approximated from the direction of incoming flow.

The time derivative is discretized analogously. In the model, the usual forward difference is used.

### 3.3 Groundwater flow

Instead of using directly the different discretization formulas, the flow equations were discretized using the control volume formulation, i.e. writing mass balance equations for a control volume and employing the principle of conservation of mass. The heterogeneities and anisotropies in the formulation could thus be more directly and easily taken into account.

Thus, using the nomenclature of Fig. 3.1, we get for the volumetric flow (m³/s):

$$\left(q_e - q_w\right) \Delta y \Delta z + \left(q_s - q_n\right) \Delta x \Delta z + \left(q_d - q_u\right) \Delta x \Delta y = Q'', \quad (3-2)$$

where the mass accumulation term $Q''$ accounts for change of mass inside the control volume. Equations for the remaining flow rate components are obtained analogously. Defining the variables:
Fig. 3.1: Discretization nomenclature.

\[ A_* = \frac{k_*}{\mu_*}, \quad \text{where } *=e,w,s,n,d,u, \quad (3-3) \]

we finally get:

\[
\begin{align*}
\left(\frac{A_e + A_w}{(\Delta x)^2} + \frac{A_s + A_n}{(\Delta y)^2} + \frac{A_d + A_u}{(\Delta z)^2}\right)P_{i,j,k} &= \\
&= \frac{A_e}{(\Delta x)^2} P_{i+1,j,k} + \frac{A_w}{(\Delta x)^2} P_{i-1,j,k} + \frac{A_s}{(\Delta y)^2} P_{i,j+1,k} + \frac{A_n}{(\Delta y)^2} P_{i,j-1,k} \\
&+ \frac{A_d}{(\Delta z)^2} P_{i,j,k+1} + \frac{A_u}{(\Delta z)^2} P_{i,j,k-1} - \frac{g}{\Delta z} (A_d \rho_d - A_u \rho_u) + \frac{Q'}{\Delta x \Delta y \Delta z}.
\end{align*} \tag{3-4}
\]

The thermal parameters at the control volume faces are obtained by direct averaging. For permeability, however, the effective values at control volume faces are obtained by considering the two adjoining permeabilities to be connected in series. Analogously with electrical resistances in parallel, we get e.g. (even grid spacing):

\[
k_e = \frac{2}{k_{xx}^i + k_{xx}^{i+1}}, \quad (3-5)
\]

where grid indexes are denoted by superscripts and \(k_{xx}\) is one of the diagonal elements in the permeability matrix Eq.(2-6).
3.4 Heat transfer

The heat transfer equation is discretized using central differences for heat conduction terms and upwind method for convective heat transport. The application of central difference formulae is straightforward. In the upwind discretization, only the convective heat transfer flowing into the node is accounted for, or

\[(\bar{q} \cdot \nabla T)_z = (q \nabla T)_w + (q \nabla T)_e,\]

where

\[(q \nabla T)_w = \begin{cases} q_w \frac{T_i - T_{i-1}}{\Delta x}, & q_w > 0 \\ 0, & q_w \leq 0 \end{cases}, \quad (q \nabla T)_e = \begin{cases} 0, & q_e \geq 0 \\ q_w \frac{T_{i+1} - T_i}{\Delta x}, & q_e < 0 \end{cases}\]

with additional subscripts dropped for clarity.

Employing forward difference for discretization in time, we then have the discretized equation for heat flow in evenly spaced grid:

\[
\frac{T_{i,j,k}^{t+\Delta t} - T_{i,j,k}^t}{\Delta t} = \frac{\lambda_k}{(\rho c)_{s,k}} \left[ \frac{T_{i,j,k}^t - T_{i-1,j,k}^t}{(\Delta x)^2} + \frac{T_{i,j+1,k}^t + T_{i,j-1,k}^t}{(\Delta y)^2} - 2 \left( \frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} \right) T_{i,j,k}^t \right] \\
+ \frac{1}{(\rho c)_{s,k}} \left[ \frac{\lambda_{kav}}{T_{i,j,k+1}^t - 2T_{i,j,k}^t + T_{i,j,k-1}^t + \frac{T_{i,j,k+1}^t - T_{i,j,k-1}^t}{2\Delta z}} \right] \\
- \frac{(\rho c)_f}{(\rho c)_{s,k}} \left[ \frac{T_{i,j,k}^t - T_{i-1,j,k}^t}{(\Delta x)} \max(q_w,0) + \frac{T_{i+1,j,k}^t - T_{i-1,j,k}^t}{(\Delta x)} \min(q_e,0) \right] \\
+ \frac{T_{i,j,k}^t - T_{i,j,k-1}^t}{(\Delta y)} \max(q_n,0) + \frac{T_{i,j+1,k}^t - T_{i,j,k}^t}{(\Delta y)} \min(q_s,0) \right] \\
+ \frac{T_{i,j,k}^t - T_{i,j,k-1}^t}{(\Delta z)} \max(q_w,0) + \frac{T_{i,j,k+1}^t - T_{i,j,k}^t}{(\Delta z)} \min(q_d,0) \right] \\
+ \frac{H}{(\rho c)_{s,k}},
\]

(3-8)
where superscript denotes time (time step \( \Delta t \)). For \((pc)_s\) and \(\lambda_k\), vertical heterogeneity (layering) is assumed. \(\lambda_{k,av}\) denotes vertically averaged thermal conductivity, approximated here, in accordance with central difference approximation, as:

\[
\lambda_{k,av} = \frac{\lambda_u + \lambda_l}{2} = \frac{\lambda_{k-1} + 2\lambda_k + \lambda_{k+1}}{4}, \tag{3-9}
\]

The explicit form of the heat source term \(H\) (\(W/m^3\)) depends on the type of heat source in use. The model includes three alternative forms of heat source: power, flow and temperature source.

With flow source, fluid at a specified temperature is injected into the porous medium. In the model, special measures had to be taken to ensure the stability of the source term. In its basic form

\[
H_f = \frac{(pc)_{src} F_{src}\left(T_{src} - T_{i,j,k}\right)}{\Delta x \Delta y \Delta z}, \tag{3-10}
\]

where subscript \(src\) denotes source and \(F\) is the flow rate (negative for discharge), stability problems are encountered with increasing time step size. The instability is caused by the assumption of constant \(\Delta T = T_{src} - T_{i,j,k}\), implicit in the source term equation (3-10). Actually, this difference decreases during a time step, thus leading to a decrease in \(\Delta T\). A better approximation is obtained by writing, instead of Eq.(3-10):

\[
H_f = \frac{(pc)_{src} F_{src}\left(T_{src} - \frac{T_{i,j,k}^t - T_{i,j,k}^{t+\Delta t}}{2}\right)}{\Delta x \Delta y \Delta z}, \tag{3-11}
\]

The implementation of the other source types is more straightforward and is described in Publication I.

### 3.5 Solute transport

The solute transport equation is discretized analogously with the heat transfer equation, using central differences for diffusion terms and upwind method for advective solute transport. Compared to heat transfer equations, concentration \(C\) replaces temperature \(T\) and actual flow velocity \(\bar{v}\) is used instead of the Darcy
velocity $\vec{q}$. Additional terms also result from the assumption of heterogeneous dispersion coefficients (Publication I).

### 3.6 Numerical dispersion

The formulae for numerical dispersion, inherent in the upwind method employing forward and backward differences (Sod, 1985), can be deduced from the Taylor series expansion. Expanding the series around a point $x_0$ (1-dimensional treatment) and truncating the series, we get e.g. for temperature gradient $T'(x)$:

$$T'(x_0) = \frac{T(x) - T(x_0)}{x - x_0} - \frac{1}{2} T''(x - x_0),$$

(3-12)

where $T''$ represents the second derivative. Comparing to the upwind term in the heat transfer equation, we see that the effect of numerical dispersion is to add a second term proportional to the second derivative of temperature. A possible method for numerical dispersion correction is thus to modify the heat conduction. Comparison of this with the heat transfer equation leads to correction factor for the dispersivity $\kappa$:

$$\kappa_{i,\text{tot}} = \left( \frac{\lambda}{(\rho c)_g} \right)_{\text{tot}} = \frac{\lambda}{(\rho c)_g} - \frac{|\vec{q}| \Delta t (\rho c)_f}{2 (\rho c)_g}, \quad i = x, y, z.$$  

(3-13)

A corresponding correction factor can also be derived for solute transport equations (Publication I).

### 3.7 Stability

As stated above, the length of time step and grid spacings cannot be chosen independently in the explicit finite difference method. An incorrect choice may lead to numerical instability (Patankar, 1980; Roache, 1976).

Also, the need for the upwind approximation and the benefits obtained when using it can be shown by performing a stability analysis on the transport equations.

One set of stability conditions may be derived using a principle of positive coefficients (Patankar, 1980). This principle states that in cases where the value of a dependent variable in a node point is influenced by the values at neighbouring grid points only through convection and conduction, an increase in the value at one grid point should, with other conditions remaining unchanged,
lead to an increase also at the neighbouring grid point. Starting from the heat transfer equation, written in a general form:

\[
a'_0 T'_{i,j,k} + a_{x1} T'_{i-1,j,k} + a_{x2} T'_{i+1,j,k} + a_{y1} T'_{i,j-1,k} + a_{y2} T'_{i,j+1,k} + a_{z1} T'_{i,j,k-1} + a_{z2} T'_{i,j,k+1}
\]

we are then lead to demand that all coefficients \( a_{nn} \) in Eq. (3-14) must have same sign. Usually, they are chosen to be positive (Patankar, 1980).

Examining first the heat transfer equation written using central differences also in the convection terms, we have by assuming further for simplicity a constant thermal conductivity \( (\lambda) \):

\[
a'_0 = \frac{1}{\Delta t}, \quad a_0 = \frac{1}{\Delta t} - 2\kappa \left( \frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} \right),
\]

\[
a_{x1} = \frac{\kappa}{(\Delta x)^2} - \frac{\xi q_x}{2\Delta x}, \quad a_{y1} = \frac{\kappa}{(\Delta y)^2} - \frac{\xi q_y}{2\Delta y}, \quad a_{z1} = \frac{\kappa}{(\Delta z)^2} - \frac{\xi q_z}{2\Delta z},
\]

\[
a_{x2} = \frac{\kappa}{(\Delta x)^2} + \frac{\xi q_x}{2\Delta x}, \quad a_{y2} = \frac{\kappa}{(\Delta y)^2} + \frac{\xi q_y}{2\Delta y}, \quad a_{z2} = \frac{\kappa}{(\Delta z)^2} + \frac{\xi q_z}{2\Delta z},
\]

\[
\kappa = \frac{\lambda}{(\rho c)_g}, \quad \xi = \frac{(\rho c)_f}{(\rho c)_g}.
\]

Because

\[
a'_0 = \frac{1}{\Delta t} > 0,
\]

we are thus lead to demand also the other coefficients to be positive, which leads to conditions (Publication I):

\[
\Delta t \leq \left[ 2\gamma \left( \frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} \right) \right]^{-1},
\]

\[
\frac{\xi |q_i| \Delta i}{\gamma} \equiv Pe \leq 2, \quad i = x, y, z.
\]
where \( Pe \) is the Peclet number. Equation (3-17) is the well-known stability condition for pure heat conduction (Roache, 1976). For example, with typical (Finnish) groundwater parameters (Iihola et al., 1987)

\[
(\rho c)_f = 4.2 \frac{MJ}{m^3K}, \quad (\rho c)_s = 3.0 \frac{MJ}{m^3K}, \quad \lambda = 2.0 \frac{W}{mK}
\]

and with \( \Delta x = \Delta y = \Delta z = 5 \text{ m} \) we have \( \Delta t \leq 1735 \text{ h} \), which generally is not a strict condition. However, from Eq.(3-18), we have with e.g. \( q = 100 \text{ m/year} \):

\[
\Delta \leq 0.3 \text{ m}, \quad \Delta = \max(\Delta x, \Delta y, \Delta z)
\]

which is a very limiting condition. Furthermore, it is independent of the length of the time step so that the problem cannot be solved by changing the time step.

By using the upwind method, and assuming first \( q_i > 0 \) \((i=x,y,z)\) we have, instead of the coefficients in Eq.(3-15):

\[
a_0' = \frac{1}{\Delta t},
\]

\[
a_0 = \frac{1}{\Delta t} - 2\kappa \left( \frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} \right) \xi \left( \frac{q_x}{\Delta x} + \frac{q_y}{\Delta y} + \frac{q_z}{\Delta z} \right),
\]

\[
a_{x1} = \frac{\kappa}{(\Delta x)^2} + \frac{\xi q_x}{\Delta x}, \quad a_{y1} = \frac{\kappa}{(\Delta y)^2} + \frac{\xi q_y}{\Delta y}, \quad a_{z1} = \frac{\kappa}{(\Delta z)^2} + \frac{\xi q_z}{\Delta z},
\]

\[
a_{x2} = \frac{\kappa}{(\Delta x)^2}, \quad a_{y2} = \frac{\kappa}{(\Delta y)^2}, \quad a_{z2} = \frac{\kappa}{(\Delta z)^2}.
\]

(3-19)

Because of the assumption of positive flow components, all coefficients except \( a_0 \) are always positive. This result is, however, independent of the assumption of positive flow rates. E.g., with \( q_x < 0 \), the upwind formulation for the x-component changes to

\[
a_{x1} = \frac{\gamma}{(\Delta x)^2}, \quad a_{x2} = \frac{\gamma}{(\Delta x)^2} - \frac{\xi q_x}{\Delta x},
\]

(3-20)

leading again to unconditionally positive coefficients \( a_{x1} \) and \( a_{x2} \). The same result is obtained also for the y- and z-components.
We thus get the stability condition:

\[
\Delta t \leq \left[ 2 \kappa \left( \frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} \right) - \xi \left( \frac{|q_x|}{\Delta x} + \frac{|q_y|}{\Delta y} + \frac{|q_z|}{\Delta z} \right) \right]^{-1}, \quad (3-21)
\]

which with the same parameters as above (\(\Delta x = \Delta y = \Delta z = 5 \text{ m} \), \(q_x = q_y = q_z = 100 \text{ m/y} \)) leads to the stability condition:

\[
\Delta t \leq \left[ 0.16 \cdot 10^{-6} + 2.7 \cdot 10^{-6} \right]^{-1} \approx 98 \text{ h} \quad . \quad (3-22)
\]

This is a more limiting condition than that obtained from Eq.(3-17) for central differences, but still manageable. On the other hand, no condition for the grid spacing alone (Eq. 3-18) is obtained. Conduction and convection parts can in this case be seen to be of same order of magnitude. Actually, however, flow rates in excess of the value used above can occur, e.g. near the injection wells in groundwater simulation, limiting the time step typically to a maximum of about 5-50h.

Another important stability criterion, reached by other stability analysis methods, is the Courant condition (Roache, 1976) which physically states that during one time step, the flow must not advance more than one grid spacing. Generalized to porous medium flow, we have

\[
\Delta t \leq \min \left( \frac{1}{\xi q_i} \right), \quad i = x, y, z \quad , \quad (3-23)
\]

where the factor \(\xi \) is needed because of the form of the convection term in the heat transfer equation resulting from the temperature equilibrium approximation. This is a less limiting stability criterion, giving with the same parameters as in Eq. (3-22) a limitation \(\Delta t \leq 312 \text{ h} \).

Figure 3.2 shows the results of simulation experiments as well as the theoretical curve (Eq. 3-21) in a case where water at the temperature of 70\(^\circ\)C is injected into a typical Finnish aquifer (natural flow rate 100 m/year) at a rate of about 10 m\(^3\)/h. The instabilities are caused mainly by the high buoyancy flows near the well. The flow velocities used in calculation of the stability conditions are actual values calculated by the program.
From Fig. 3.2, it can be seen that the Courant condition is necessary but not sufficient, whereas Eq.(3-21) is sufficient but not necessary condition for stability.

The stability equations for solute transport can be deduced analogously with those for heat transport (Publication I). We get:

\[
\Delta t \leq \left[ \frac{2D}{R} \left( \frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} \right) + \frac{1}{R} \left( \frac{|v_x|}{\Delta x} + \frac{|v_y|}{\Delta y} + \frac{|v_z|}{\Delta z} + \lambda_d \right) \right]^{-1}, \tag{3-24}
\]

\[
\Delta t \leq \min \left( R \frac{\Delta i}{|v_i|} \right), \quad i = x, y, z, \tag{3-25}
\]

\[
\frac{D_{i+1,j,k} + D_{i-1,j,k}}{D_{i,j,k}} \leq 4 \quad \text{(analogously for y and z directions)}, \tag{3-26}
\]

where \( D \) the dispersion coefficient, \( v_i \) are the actual flow velocity components (\( v_i = q_i/n \)), \( \lambda_d \) is the radioactive decay constant and \( R \) is a retardation coefficient. The second inequality is the Courant condition, whereas the last condition results from the heterogeneity of the dispersion coefficient. Sudden and large spatial changes in dispersion factor may thus cause instability.

For a typical case, by choosing in addition to the parameters used in inequalities
(3-21) and (3-22) arbitrary representative values:

$$D = 3 \cdot 10^{-9} \frac{m^2}{s}, \quad \lambda_d = 7.3 \cdot 10^{-10} \frac{1}{s}, \quad R = 2, \quad n = 0.3$$

($D$ and $\lambda_d$ represent values for $^{137}$Cs: Peltonen et al., 1985; Tchobanoglous and Schroeder, 1985) we get from Eq.(3-24)

$$\Delta t \leq \left[3.6 \cdot 10^{-10} + 2.7 \cdot 10^{-6} + 7.3 \cdot 10^{-10}\right]^{-1} s = 102 h.$$

In this case, the advection part can be seen to be the most determining stability factor. However, with decreasing half-life, the radioactive decay becomes more important. E.g., with a half-life of 70 h, we have $\lambda_d = 2.75 \cdot 10^{-6} 1/s$, which is comparable to advection term in the stability condition above.

A full stability analysis is a very complicated process (Sod, 1985; Roache, 1976) and was beyond the scope of this thesis. The analysis presented above was aimed to give a simplified set of stability conditions, which can be used in the simulation model to generate a warning of possible instabilities.
4 SIMULATION MODEL THETA

4.1 Basic assumptions

On the basis of the equations presented above, a computer simulation model THETA has been developed (Publications I and II). The basic structural assumptions and limitations of the model are:

- **Zone of saturation only.** THETA simulates the flow in the zone of saturation, where all pores are filled with fluid. In case of aquifers, infiltration of water from the ground to the aquifer zone is thus not calculated.

- **Incompressible flow.** The flow equations are deduced for an incompressible fluid flowing in the porous matrix.

- **No free water surface calculation.** The information about the free water surface is contained in the pressure values. The location of free surface is not, however, calculated, and the flow takes place through all areas with non-zero permeability. As to groundwater, the program thus simulates a pressurized aquifer. With phreatic aquifers, it is thus assumed that the changes in water surface level are small.

- **General source terms.** The sources and sinks are implemented in the model directly using the source terms as described in the simulation equations: no specific well equations are used. Different types of sources can, however, be specified as described in Publication I.

- **Temperature equilibrium.** In the heat transfer calculation, a temperature equilibrium is assumed, meaning that the flowing fluid and porous matrix are described by the same temperature. This assumption has been elaborated in Chapter 2.

- **Retardation assumption.** The solute transport is calculated using the retardation assumption (Javandel et al., 1984) together with radioactive decay.

Other, more easily removable assumptions included in the code are:

- **Constant heat capacity.** The heat capacity of the solid matrix is assumed to be constant.
• *Flowing fluid is water*. The constitutive equations expressing the temperature dependency of fluid density and viscosity included in the model are for water.

### 4.2 Model structure and operation

The model solves pressure (flow), temperature and concentration distributions in 3-D grid with even grid spacings. An arbitrary number of sources can be located anywhere in the grid, except at the boundaries. The source points are grouped to a well-type structure (Fig. 4.1), in which a specified number of vertically adjacent points at a certain horizontal location forms a well. Each well can be used both for charging and discharging with independently varied injection and withdrawal rates. The grid size is not automatically chosen, but must be supplied by the user.

In the simulation, the different fields (pressure, flow, temperature, concentration) are solved at each grid point. Water flow velocities used in heat and solute transport simulation are calculated using Darcy's law with pressure values from the basic grid. In effect, flow field is thus determined using staggered grid (Patankar, 1980). In this method, the flow components are calculated at the points that lie on the faces of the control volumes and not in the grid points themselves. This enables a more accurate description of convection and advection.

Permeability can be defined to be both anisotropic and heterogeneous. Totally heterogeneous and anisotropic permeability is defined by a matrix, which contains a permeability value for each grid point separately. In an anisotropic case, separate matrixes for all the principal directions (x, y and z) are needed as input. A simpler input format is provided to ease the definition of permeability in case of layered porous media (e.g. aquifers in many cases), where heterogeneities

![Fig. 4.1: Source definition. Black dots represent well screens.](image)
are present in vertical direction only.

Program structure is visualized in Fig. 4.2 The detailed program control takes place in subroutine AQSTOR, which controls the actual porous medium calculation. The main program THETA, on the other hand, controls the simulation as a whole. Because the nearly independent function of AQSTOR, THETA can easily be replaced by another program with different control. In this way, the porous medium calculation routines can be connected as an independent part to a larger program, e.g. an energy system model (Publication IV).

In the simulation, the pressure equations are first solved iteratively to find the stationary flow field corresponding to prevailing temperature and concentration values and source terms. The changes in temperature and concentration fields are the calculated time step by time step using the flow rates thus obtained. At user defined intervals, a new stationary flow field is calculated. The frequency of numerical stability checks and printouts is also user defined.

Simulation input data consists of several files, the two main files defining the simulation control and numerical input as well as source locations. Additional files can be used in case of more complicated input data, like heterogeneous permeability or groundwater surface elevation data. As output, the temporal and spatial distribution of various variables (pressure, potential, flow, temperature, concentration) can be printed out in various forms. Heat balance as well as

![Program structure diagram](Image)

**Fig. 4.2 : Program structure.**
source/sink temperatures and concentrations can also be printed out. Model input and output are described in detail in Publication I.

4.3 User interface

To enhance model usability and user convenience, a graphic user interface for the PC environment has been developed (Publications I and II). The interface enables interactive input data definition as well as on-line visualization of simulation results. The interface has been coded using Lahey Fortran graphic extensions.

The user interface consists of a menu and an on-line part, the menu part giving the user the ability to define input/output files and the on-line part visualizing the advance of simulation.

During the simulation, two types of screens are available (Fig 4.3). The first of the screens is intended to give numerical data about the most important simulation variables, whereas the second screen gives a more qualitative picture of the simulation process by displaying temperatures or concentrations graphically in a user defined two-dimensional cross section. The user can switch between these screens at will during the simulation.

To some extent, the user can influence the data shown on the screen by input data or interactively during the simulation. A more detailed description of the on-line graphics can be found from Publications I and II.

4.4 Supplementary programs and routines

4.4.1 Energy system simulation

When utilizing energy stored in an aquifer, a whole energy system capable of extracting heat from the aquifer and of transferring it to the load is needed. In addition, some means of injecting heat into the aquifer must be provided. The exact configuration of an energy system varies with different applications. There are, however, some basic elements that are common to different applications and with which an energy system for desired use can be formed.

To enable energy system simulations, a special version of THETA called AQSYST (publication IV) has been developed. This has been accomplished by connecting the porous medium subroutines to an energy system model based on earlier work by Lund (1987). The following subsystems were included in the model:
Simulation

<table>
<thead>
<tr>
<th>Step</th>
<th>10 of 600</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hour</td>
<td>10</td>
</tr>
<tr>
<td>Day</td>
<td>1</td>
</tr>
<tr>
<td>Year</td>
<td>1</td>
</tr>
<tr>
<td>Left</td>
<td></td>
</tr>
</tbody>
</table>

Temperatures

<table>
<thead>
<tr>
<th>Id</th>
<th>Coord.</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Well 1</td>
<td>averaged</td>
<td>71.8 DegC</td>
</tr>
<tr>
<td>Well 2</td>
<td>averaged</td>
<td>6.7 DegC</td>
</tr>
<tr>
<td>Loc 0</td>
<td>8,6,5</td>
<td>14.8 DegC</td>
</tr>
<tr>
<td>Loc 1</td>
<td>8,7,5</td>
<td>40.9 DegC</td>
</tr>
<tr>
<td>Loc 2</td>
<td>8,8,5</td>
<td>14.1 DegC</td>
</tr>
<tr>
<td>Loc 3</td>
<td>8,9,5</td>
<td>7.8 DegC</td>
</tr>
</tbody>
</table>

Energy balance

| Ten in | 71.8 DegC |
|        | DegC      |
| TOT IN | 0.32E+11 J|
| OUT    | 0.00E+00 J|
| Rec.F. | 0.0 %    |

Control

<table>
<thead>
<tr>
<th>Subr</th>
<th>TRANSP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iter</td>
<td>3</td>
</tr>
<tr>
<td>--inc</td>
<td>0.896</td>
</tr>
</tbody>
</table>

Logo

Ave in : 0.900E-00
Ave out: 0.000E+00

Concentration flows

| Ave in | 13.3 m3/h |
| Ave out| 8.8 m3/h  |

Well flows

| Ave in | 13.3 m3/h |
| Ave out| 8.8 m3/h  |

Fig. 4.3: On-line graphic screens (gray-scaled).
- storage (aquifer)
- heat pump
- buffer water storage
- boiler (electric or oil-fired)
- heat load
- heat source

As to heat source, the charging modes include:

- continuous heat source with constant temperature
- yearly heat pulse with constant temperature and arbitrary duration
- lake water with sinusoidally varying temperature
- solar collectors

Each subsystem is described as a 'black box' with a certain set of input and output values. The input depends on subsystem connections, output being mainly determined by system physics. Subsystem control is also important, having in some cases crucial effect on system performance and dynamics. In addition, different kind of limitations on parameter values as well as external factors such as solar radiation and ambient temperature are taken into account in subsystem simulation.

The subsystems are linked together using a connection matrix describing the existence and nature of the links between the subsystems. Figure 4.4 shows one possible system configuration supplying heat for a residential load. The aquifer

![Diagram of system configuration](image)

Fig. 4.4 : Typical system configuration for AQSYST.
acts in this case as a low-temperature seasonal heat storage. It not only stores the heat but transports it from the heat source to the heat load. Different types of energy systems can be constructed by connecting these subsystem models in a desired way.

4.4.2 Permeability matrix generation by Markov processes

The definition of permeability distribution in case of heterogeneous permeability is a complicated process, because it involves writing down a matrix containing a numeric value for each grid point. An heterogeneous permeability matrix may be encountered e.g. when simulating ground with fracture zones. The process is even more complicated in case of anisotropic permeability, when matrixes for all three principal directions must be provided. The amount of work grows rapidly with increasing grid dimensions.

A further complication is the acquisition of data needed for permeability matrix. Exact permeability data is scarcely available, and even with the available data, uncertainties as to numeric values may be great, in the worst case even several orders of magnitude.

The generation of permeability data can be eased by using some procedure to generate the full data set from a limited amount of initial knowledge. The processes involved in the formation of stratigraphic sequences may, however, be so complex that it is difficult to write deterministic functional relationships to represent the processes. As an alternative, probabilistic relationships can be employed in many applications.

The stochastic method of generating stratigraphic sequences is based on the fact that transitions between successive bedding units are dependent on the earlier history of the layer formation. Thus, for example, the probability of deposition of a coal bed may depend e.g. whether an underclay was deposited in the earlier event (Harbaugh and Merriam, 1968). In this case, a “memory” effect is present and the process is commonly referred to as a Markov process.

With Markov processes, the memory effect is described by a matrix of probability values that specify the transformation from one state to another. Referring to Table 4.1 describing a three-state system, $P_{11}$ is the probability of clay layer following another clay layer, $P_{32}$ the probability of finding a sand layer after a gravel layer etc. Same type of matrix can also be defined for the layer thickness frequency distribution.
Table 4.1: Transition matrix for a Markov process.

<table>
<thead>
<tr>
<th></th>
<th>clay</th>
<th>sand</th>
<th>gravel</th>
</tr>
</thead>
<tbody>
<tr>
<td>clay</td>
<td>$P_{11}$</td>
<td>$P_{12}$</td>
<td>$P_{13}$</td>
</tr>
<tr>
<td>sand</td>
<td>$P_{21}$</td>
<td>$P_{22}$</td>
<td>$P_{23}$</td>
</tr>
<tr>
<td>gravel</td>
<td>$P_{31}$</td>
<td>$P_{32}$</td>
<td>$P_{33}$</td>
</tr>
</tbody>
</table>

For THETA, a utility routine for defining the permeability matrix in three dimensions using the Markov process approach described above has been developed (Lundström, 1988). Not only heterogeneity, but also anisotropic permeability distribution can be generated. In the simulations presented in the thesis, the Markov method was not, however, utilized.

With the program, the matrix directly can also be generated directly from user-specified information about the permeability distribution, with no stochastic calculation. This property of the program can be used e.g. to generate fracture zones of known permeability and direction in an otherwise homogeneous solid matrix. This method was utilized in the nuclear waste simulations.

### 4.4.3 Output routines

In addition to on-line graphics, special output routines have been developed to aid in the manipulation of the simulation results. These include utility programs for converting the program output to be used by special graphics routines for visualizing temperature or concentration contours and flow field. In the main frame computer environment, DISSPLA graphics library based programs for data visualization have been developed.

### 4.5 Program performance and requirements

The program code is written using FORTRAN language conforming to the '77' standard, the model thus being applicable in various platforms ranging from PC's to super computers. The main body of the program comprises about 11000 lines, with an additional about 5000 lines in the supplementary and utility programs.

On a PC, the following software/hardware is needed to run the program:

- 80386 or later compatible processor with a coprocessor
- DOS operating system, version 5.0 or later
- 1 MB of core memory (2 MB or more recommended)
- Microsoft compatible mouse (on-line graphics)
• VGA display and a video board with at least 1MB of memory
• 350 kB of hard disk space (for the program; additional 100 - 1000 kB needed for the input and output data)

On a main frame computer environment, THETA has been tested in UNIX (AIX) and VM operating environments. The need for core memory and disk space is dependent on the specifics of the operating system, being mostly over 2-3 MB.

The program performance on different platforms has been evaluated by simulating a reference case (the Rajamäki hot water experiment), which consists of about 4 month injection of hot water (70°C) into an aquifer at an original temperature of 6°C. The simulation area consisted of 4356 grid points and 792 time steps (1 h) were needed to cover the desired time period. Figure 4.5 shows a comparison of the CPU requirement on different platforms. As can be seen, the simulation time ranges from the 50 minutes on the earliest used PC platforms to about 2 minutes on Pentiums and to 6 seconds on a Cray supercomputer.
5 MODEL VERIFICATION

The proper function of the model equations was verified by simulating some simple cases, for which an analytical solution could be found. The simulated cases were chosen to represent typical cases in the main field of model application, i.e. aquifer thermal energy storage; an extensive numerical analysis was not made. The cases included 1-dimensional heat conduction and conduction+convection, 3-dimensional (radial symmetry) heat conduction as well as 1-dimensional solute transport.

5.1 1-dimensional heat conduction

To verify the heat conduction part of the equations, a 1-dimensional case of pure heat conduction was first studied. The governing equation in this case is:

\[ \frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2} \quad \kappa = \frac{\lambda_g}{(\rho c)_g} \quad (5-1) \]

where \( \kappa \) is thermal dispersivity. In a semi-infinite solid, and with boundary conditions

\[ T(x,0) = 0 \]
\[ T(0,t) = T_0 \quad t > 0 \quad (5-2) \]

the solution to this problem is (Carslaw and Jaeger, 1986):

\[ \text{Fig. 5.1: 1-dimensional heat conduction: temperature at a distance of 5 m.} \]
\[ T = T_0 \text{erfc}\left(\frac{x}{2\sqrt{\kappa t}}\right) \]  

(5-3)

where \( \text{erfc} \) is the complementary error function.

The one-dimensional simulation was accomplished in THETA by defining a grid with dimensions of only 3 grid points in directions perpendicular to the flow. The outermost points formed the surface, across which non-conductive and no-flow boundary conditions were maintained. The hydraulic gradient was set zero and permeabilities to very small values to guarantee no-flow condition also inside the simulated domain. Time step was 1 hour and grid spacing 0.5 m.

Figure 5.1 shows the temperature at a distance of 10 grid points (5 meters) from the boundary which was kept at 70°C. The initial temperature in the calculation domain was 0°C, and the dispersivity had a typical aquifer value \( \kappa = 0.67 \times 10^{-6} \) m²/s. As can be seen from the figure, the analytical and simulated temperatures match very well.

### 5.2 1-dimensional heat conduction and convection

The one-dimensional coupled heat conduction and convection is governed by equation:

\[
\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2} \frac{(pc)_f}{(pc)_g} \frac{\partial T}{\partial x} + \kappa = \frac{\lambda_g}{(pc)_g} \quad (5-4)
\]

where the subscripts \( f \) and \( g \) refer to fluid and fluid saturated solid matrix, as before. In this case, applying boundary conditions

\[
T(x,0) = T_0 \\
T(0,t) = T_1, \quad t > 0 \quad (5-5)
\]

the solution is (Carslaw and Jaeger, 1986):

\[
T = T_0 + \frac{1}{2} \left[ T_1 - T_0 \right] \left[ \text{erfc}\left(\frac{x-Ut}{2\sqrt{\kappa t}}\right) + e^{\frac{U_x}{2\sqrt{\kappa t}}} \text{erfc}\left(\frac{x+Ut}{2\sqrt{\kappa t}}\right) \right] + \frac{(pc)_f}{(pc)_g} q \quad (5-6)
\]
Fig 5.2: 1-dimensional heat conduction and convection: temperature at
a) distance 10 m, q = 6 m/year; b) distance 25 m, q = 50 m/year;
c) distance 50 m, q = 200 m/year.
The case was simulated 1-dimensionally by THETA as described above. The same grid spacing as above (0.5 m) was used. Figure 5.2a shows the analytical and simulated temperatures at the distance of 20 grid points (10 meters) without and with numerical dispersion correction. The specific discharge was about 6 m/year. As can be seen from the figure, the simulated values overshoot slightly (1.5 °C after one year) the analytical values. By including numerical dispersion correction, the amount of overshoot is decreased to 0.3 °C.

With increased flow rate (Figs. 5.2 b and c), the fit remains fairly good, although the effect of numerical dispersion is more pronounced. It can also be seen that with high enough flow rate, the application of the numerical dispersion correction based on equation (3-13) leads to oscillations, which inhibits the use of the numerical dispersion correction of this form with high flow rates. Decreasing the grid spacing to half in the case depicted in Fig. 5.2c lead to only small decrease in numerical dispersion.

5.3 Radial heat conduction

In three dimensions, the heat conduction equation with constant parameters can be written as:

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T \quad , \quad \kappa \equiv \frac{\lambda_g}{(\rho c)_g} (5-7)$$

If heat is liberated at a constant rate of $\Phi(\rho c)_g$ per unit time at a point inside the medium from $t=0$ onwards, the solution to the equation with initial temperature set to $T_0 = 0$ is (Carslaw and Jaeger, 1986):

$$T = \frac{\Phi}{4\pi \kappa r} \text{erfc} \left( \frac{r}{\sqrt{4\kappa t}} \right) (5-8)$$

where $r$ is the distance from the source point and $\text{erfc}$, as before, the complementary error function. The case was simulated with THETA in a 40x40x40 grid, with the source point (100 W) in the middle. The grid spacing was 0.1 m and time step 0.5 hours. Fig 5.3 shows the development of temperature at a distance of 1 meter (10 grid points) as a function of time. The total simulation time was 500 hours. The fit can be seen to be good, maximum difference in the temperature being 0.3°C.
The overshooting of temperatures at early times in the simulation is caused by discretization: the first effects of the heat pulse advance faster through the 10 grid points (or elementary volumes) than they do in analytical solution. The decrease in the simulated temperature below the analytical value at the end of the simulation is at least partly caused by the rear boundary, which was kept at a constant temperature (initial value 0°C). Because of the small grid spacing, an unreasonably large grid would have been necessary to prevent the thermal interaction between the advancing heat front and the rear boundary.

5.4 1-dimensional solute transport

In solute transport, the solution of equation (constant parameters)

$$\frac{R \partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - \nu \frac{\partial C}{\partial x} - \lambda_d C R$$

(5-9)

with a constant concentration at the front boundary and the initial concentration set at 0, or

$$C(x,t) = 0 \text{ when } t = 0$$

$$C(0,t) = C_0 \text{ when } t > 0$$

(5-10)

has a solution (Javandel et al., 1984)
Fig 5.4: 1-dimensional solute transport: relative concentration at a distance of 10 meters a) in base case; b) with a smaller grid spacing; c) with numerical dispersion correction.
\[
\frac{C}{C_0} = \frac{v}{v+U} \exp \left[ \frac{x(v-U)}{2D} \right] \text{erfc} \left[ \frac{Rx-Ut}{2\sqrt{D\gamma t}} \right] \\
+ \frac{v}{v-U} \exp \left[ \frac{x(v+U)}{2D} \right] \text{erfc} \left[ \frac{Rx+Ut}{2\sqrt{D\gamma t}} \right] \\
+ \frac{v^2}{2DR\lambda_d} \exp \left[ \frac{\nu x}{t} - \lambda_d \right] \text{erfc} \left[ \frac{Rx+vt}{2\sqrt{D\gamma t}} \right], \quad U = \sqrt{v^2 + 4DR\lambda_d}.
\]

(5-11)

The equation was solved both analytically and numerically using the parameters:

\[
D = 3 \cdot 10^{-9} \frac{m^2}{s}, \quad \lambda_d = 7.3 \cdot 10^{-10} \frac{1}{s}
\]

(5-12)

\[
R = 2, \quad v = 4.47 \cdot 10^{-6} \frac{m}{s}
\]

The value of the dispersion coefficients vary widely; the value used here represents a typical value in groundwater flow (Peltonen et al., 1985; Tchobanoglous and Schroeder, 1985). Values for the retardation factor and groundwater flow are typical ones in groundwater hydrology and are not intended to represent any specific conditions or species. For the radioactive decay constant, the value for \(^{137}\text{Cs}\) was used.

In the simulation, grid spacing was 0.5 m and time step 1h. Figure 5.4a shows the relative concentration \((C/C_0)\) as a function of time at a distance of 10 meters from the constant concentration boundary. The effect of numerical dispersion in the simulation can be clearly seen as an earlier and slower rise of the concentration at the specific location. By decreasing the simulation grid spacing, a better agreement is obtained, as shown Fig. 5.4b which illustrates the results of a simulation where the grid spacing was reduced to one half.

The effect of numerical dispersion can also be reduced by using the numerical dispersion correction factor (Publication I). Care must be exercised, however, as it was found that by applying the correction described in Eq.(73) in Publication I does improve the agreement in the slope of the concentration curve, but at the same time induces oscillations (Fig. 5.4c). By applying only 50\% of the correction factor, no oscillations are induced and the resulting curve is almost identical to the one in Fig. 5.4b.

In all, the verification runs indicated that the effect of numerical dispersion is much more pronounced in the case of solute transport than in heat transport. Every effort must thus be made to use as small grid spacing as possible in the simulations.
6. MODEL VALIDATION

The correct performance of the simulation model THETA was validated using experimental data obtained from three different aquifer heat storage field experiments. The experiments were chosen to represent a wide variety of storage charge/discharge as well as geometrical parameters. The experiments were not, however, designed for the purpose of validation of THETA, but had been conducted earlier for various purposes. Two of the experiments were conducted in Finland and one in Switzerland.

6.1 Aquifer thermal energy storage

In an aquifer thermal storage, the groundwater saturation zone is used for heat storage purposes. Fig. 6.1a shows the system principle. In charging phase, hot water is injected into the aquifer through a well drilled into the water containing formations. At the recovery phase, flow is reversed and the stored water is pumped out of the aquifer. To prevent any unwanted chemical reactions in the aquifer, a closed cycle is usually maintained, the water injected into the aquifer taken from some other part of the same aquifer and heat transfer to source or load taking place via a heat exchanger.

The basic single-well system (also called two-well system, because usually a closed system is maintained, as mentioned above) depicted in Fig. 6.1a is applicable only in aquifers with very small groundwater flow rates. More generally, heat is transferred away from the injection well by groundwater flow, and two groups of wells must be used, one for heat injection and another for heat recovery. In this kind of multi-well system (Fig. 6.1b), heat is injected into the aquifer through one well system and recovered at a later time through separate wells lying downstream of the injection wells. The emphasis in this study was on multi-well systems, although the model itself can be applied in both cases.

The single-well storage is the most used configuration in aquifer storage applications. The geological conditions in some countries, e.g. in the Nordic countries, favour high-flow gravel-based esker aquifers for which a multi-well configuration is needed. The natural flow rates in esker aquifers can be as high as 0.5-1 km/year, compared to 0-20 m/year of the more stationary aquifers. Experiments show that aquifer thermal energy storage is technically feasible also in these high-flow conditions (Iihola et al., 1987).

The basic figures of merit describing an aquifer heat storage used in the verification to compare measured and simulated behaviour were extraction
temperature and energy recovery ratio ($\eta$), the latter being defined as the ratio of the heat recovered from the storage to the injected energy:

$$\eta = \frac{Q_{out}}{Q_{in}} = \frac{C_{out} V_{out} (T_{out} - T_{ref})}{C_{in} V_{in} (T_{in} - T_{ref})}$$

(6-1)

where $C$ is the volumetric heat capacity, $V$ the water volume and $T$ the temperature. $T_{ref}$ is a reference temperature, which was here taken to be the natural temperature of groundwater. Subscripts $in$ and $out$ refer to storage charge and discharge, respectively.
The choice of the reference temperature is arbitrary, as long as the definition of Eq.(6-1) remains meaningful. For instance, a choice of $T_{\text{ref}} = T_{\text{in}}$ would lead to zero denominator. The choice made here (i.e. undisturbed groundwater temperature) is a natural one, as we are trying to determine the benefit of raising the groundwater temperature above its natural value. If a heat pump is utilized in the extraction process, care must be exercised in the calculation of storage efficiency, because heat pump can lower the temperature of the extracted water below its undisturbed (natural) value, leading to efficiencies in excess of 100%.

In addition to extraction temperature and energy recovery ratio, the ground temperature distribution was compared (Publication III). A disadvantage in the comparison is, however, that the temperature distribution in the ground is difficult to measure, resulting in inaccuracies in the temperature field.

### 6.2 Rajamäki high temperature experiment

Both Finnish field experiments took place at Rajamäki in southern Finland. The aquifer in question is a phreatic esker aquifer, a ridge of glaciofluvial sand and gravel formed during the last glaciation by melt water. The water carried and graded rock debris (moraine) from the ice and deposited it in the sea that covered the southern part of Finland after the glacial period. The esker is surrounded by silt and clay, which later settled in the water.

The thickness of the layer of sand and gravel deposits between the bedrock and ground level varies between 20 and 40 metres, of which 8-20 metres lies below the groundwater table. Hydraulic conductivity in the main stream of the aquifer is on the average $4 \cdot 10^3$ m/s and the hydraulic gradient 0.3-0.65 %, giving rise to a groundwater flow of 450-800 metres/year. The annual mean temperature is $+6^\circ$C and annual rainfall 600 mm, of which snow 100-150 mm. The area is covered

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>groundwater zone permeability</td>
<td>$1.2 \cdot 10^{10}$ m$^2$</td>
</tr>
<tr>
<td>aquifer volumetric heat capacity</td>
<td>2.9 MJ/m$^3$K</td>
</tr>
<tr>
<td>aquifer thermal conductivity</td>
<td>2.0 W/Km</td>
</tr>
<tr>
<td>hydraulic gradient</td>
<td>0.04 %</td>
</tr>
<tr>
<td>heat transfer coefficient to amb. air</td>
<td>0 W/m$^2$K</td>
</tr>
<tr>
<td>time step</td>
<td>4 h</td>
</tr>
<tr>
<td>horizontal grid spacing (flow dir.)</td>
<td>4 m</td>
</tr>
<tr>
<td>horizontal grid spacing (perp.to flow)</td>
<td>6 m</td>
</tr>
<tr>
<td>vertical grid spacing</td>
<td>1 m</td>
</tr>
</tbody>
</table>
and annual rainfall 600 mm, of which snow 100-150 mm. The area is covered with snow for 5 months of the year.

The high temperature experiment lasted for 4 months and took place on a more stagnant part of the Rajamäki aquifer, aside from the main stream, with a very small hydraulic gradient and a flow rate of only about 10 m/year (Publication III).

![Recovery and injection](image)

**t = 10 d**

![Recovery and injection](image)

**t = 50 d**

Fig. 6.2: Horizontal temperature distribution in the ground 10 and 50 days from the start of injection. Natural flow 10 m/y in the positive y-direction.
The aquifer itself was layered, consisting vertically of layers with different permeability. In the experiment, hot water at 70°C was injected into the aquifer and simultaneously recovered through a well located about 15 metres downstream. The main purpose was not, however, energy storage but to measure the possible chemical and biological effects of heating the groundwater.

The experiment was simulated by introducing a layered (vertically heterogeneous) permeability in the model, as suggested by the measurements (Publication III). The changes in groundwater level were assumed to be small enough to be neglected. The most important simulation parameters are shown in Table 6.1. As to heat transfer coefficient from the ground surface to ambient air, a value zero was used as it was found to have no noticeable effect on the results.

Figure 6.2 shows the simulated temporal development of temperature profile in a horizontal cross section at the upper level of well screens. This coincides with the depth above which the ground consists of less permeable materials than gravel. The spreading of the heat pulse can clearly be seen. The profile is not, however, fully symmetrical because the recovery well prevents the heat from advancing downstream and causes a more sharply rising temperature front in the downstream side. The natural groundwater flow rate is too small to cause a noticeable effect in Fig.6.2.

The vertical temperature profile is illustrated in Fig. 6.3, which shows a cross section of the ground two days after the beginning of the injection. The layering caused by buoyancy can be seen in the figure. Because of its smaller density, hot
water tends to rise up until it reaches the water surface or less permeable layer, which forces the flow to horizontal direction. The result of all this is a "tilting" (Hellström et al., 1979, Doughty et al., 1982) of the boundary between the hotter and colder region in the ground. The natural flow of the groundwater still enhances the tilting effect. In the case studied here, the natural flow was quite small and contributes only little to the tilting effect.

The buoyancy effect is also clear in the flow field, illustrated for the same cross section in Fig. 6.4. The natural flow in the figure is from left to right. The injection causes a disturbance in the flow field, forcing the flow to turn partially back. Because of buoyancy, the resulting flow pattern has the backward flow near the surface. The extraction well also disturbs the flow field, diverting even the flow in the downstream side towards it.

As to comparison with experimental data, Fig. 6.5 shows the measured and simulated recovery temperature as a function of time. The general correspondence is good, the final temperature differing by about 1°C. In the beginning, there is, however, a considerable difference in temperature (4.5°C at the largest), the simulated temperature rising slower than was observed in the measurements.

The cause for the slower temperature increase in the simulation is not clear, although there are several possible explanations. First of all, the approximation of continuous media by a finite number of grid points causes some averaging which more or less smoothes out any sudden changes. The initial state of the aquifer was also not accurately. One possible explanation is that the drilling and backwashing associated with the well construction broke the ground structure in the vicinity of the drill hole, resulting in a higher permeability. The onset of injection the might then have moved and sorted the rock debris and pebbles with
a decrease in permeability. This kind of behaviour would explain the peak observed in the recovery temperature. Unfortunately, the experimental field is not any more in use making it impossible to conduct any additional experiments.

The measured and simulated recovered recovery ratios were 54% and 57%, respectively. This is a good agreement, as it corresponds to a difference of only about 1°C in the average recovery temperature (Publication III). As can be seen from the temperature contours, the water with highest temperature is flowing above the extraction well screen. If this kind of system is to be used as a heat storage, better results would be obtained by locating the well screen higher.

As to temperature contours (Publication III), the form is the same in both experiment and simulation, but in the downstream side, the simulated contours seem to stretch further away from the wells. There are, however, much uncertainties involved, especially in deducing the contours from measurements, so the general agreement can be considered to be fair.

Table 6.2 includes a sensitivity analysis for Rajamäki hot water experiment. The location of the wells can be seen to be a sensitive parameter. Also the value of permeability, which is one of the most difficult aquifer parameters to measure, has a pronounced effect on the recovery ratio. With the uncertainties inherent in parameter measurements, the compatibility obtained in the validation can be considered to be good.
Table 6.2: Sensitivity analysis (Rajamäki experiments).

<table>
<thead>
<tr>
<th>Property</th>
<th>low temp.exp.</th>
<th>high temp.exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>change</td>
<td>change</td>
</tr>
<tr>
<td>(reference)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>hydraulic gradient</td>
<td>+20%</td>
<td>+20%</td>
</tr>
<tr>
<td>permeability</td>
<td>+20%</td>
<td>+20%</td>
</tr>
<tr>
<td>aq. thermal conductivity</td>
<td>+20%</td>
<td>+20%</td>
</tr>
<tr>
<td>aq. heat capacity</td>
<td>+20%</td>
<td>+20%</td>
</tr>
<tr>
<td>discharge well lower</td>
<td>2 m</td>
<td>1 m</td>
</tr>
<tr>
<td>discharge well higher</td>
<td>2 m</td>
<td>1 m</td>
</tr>
<tr>
<td>(reference)</td>
<td>64.4</td>
<td>57.4</td>
</tr>
<tr>
<td>hydraulic gradient</td>
<td>63.6</td>
<td>57.8</td>
</tr>
<tr>
<td>permeability</td>
<td>63.1</td>
<td>48.5</td>
</tr>
<tr>
<td>aq. thermal conductivity</td>
<td>62.7</td>
<td>56.3</td>
</tr>
<tr>
<td>aq. heat capacity</td>
<td>63.1</td>
<td>53.7</td>
</tr>
<tr>
<td>discharge well lower</td>
<td>61.0</td>
<td>53.2</td>
</tr>
<tr>
<td>discharge well higher</td>
<td>66.1</td>
<td>65.7</td>
</tr>
</tbody>
</table>

6.3 Rajamäki low temperature experiment

In the low temperature experiment (Publication III), the test area consisted of the main body of the Rajamäki aquifer, with an average groundwater flow rate of 600 m/year. The groundwater flows in a layer of sandy gravel, with water surface at about 20 meters below the ground surface.

Since 1974, cooling water from a nearby factory has been injected into the aquifer at an average temperature of 23°C (13°C - 32°C) with an average infiltration rate of 1200 m³/day. The yearly average natural groundwater temperature was 5°C (4.6°C - 5.6°C). The experiment lasted for over 10 years. In the validation, only the first eight years for which there was more detailed measured data, were considered.

Table 6.3: Low temperature experiment simulation

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>groundwater zone permeability</td>
<td>$6.1 \cdot 10^{-10}$ m²</td>
</tr>
<tr>
<td>aquifer volumetric heat capacity</td>
<td>2.9 MJ/m³K</td>
</tr>
<tr>
<td>aquifer thermal conductivity</td>
<td>2.0 W/Km</td>
</tr>
<tr>
<td>hydraulic gradient</td>
<td>0.475 %</td>
</tr>
<tr>
<td>monthly groundwater temperature</td>
<td>4.5 - 5.6°C</td>
</tr>
<tr>
<td>heat transfer coefficient to amb. air</td>
<td>0 W/m²K</td>
</tr>
<tr>
<td>time step</td>
<td>12 h</td>
</tr>
<tr>
<td>horizontal grid spacing (flow dir.)</td>
<td>15 m</td>
</tr>
<tr>
<td>horizontal grid spacing (perp.to flow)</td>
<td>15 m</td>
</tr>
<tr>
<td>vertical grid spacing</td>
<td>2 m</td>
</tr>
</tbody>
</table>
In the simulations (Table 6.3), the presence of groundwater surface was approximated by having layers with zero permeability between the ground and water surfaces. This replacement of an actually phreatic aquifer with a confined

Fig. 6.6: Advancement of heat during the first year. Natural flow 600 m/year in the positive y-direction.
one was considered acceptable, as the possible changes in groundwater surface level can be considered to be small compared to the overall dimensions of the problem. As to heat transfer coefficient, it was found by trial simulations that it had only very marginal effect on the results, so a value zero was chosen as in the high temperature experiment simulations.

Figure 6.6 shows the advancement of the heat pulse in a horizontal cross section at the top of the groundwater zone. A clear reduction in the temperature level can be observed, as was suggested also by the measurements. The increase in the temperature at the charge location is caused by variations in the injection temperature.

Compared to the average injection temperature of 23°C, the average recovery temperature for the first eight years was only 12°C. If the aquifer is to be utilized
as a heat storage, a heat pump or some other means of raising the temperature level is thus needed.

A better storage performance could also be obtained by locating the extraction wells higher, as suggested by Fig. 6.7, which shows the temperature contours in a vertical cross section containing the injection and extraction wells. With the high groundwater flow, the tilting effect can be seen to be now very pronounced.

As to comparison of simulation and measurements, Fig. 6.8 shows the recovery temperature as a function of time. The general trend is the same, but the simulated results now show an even more averaged behaviour than in the hot water experiment (maximum temperature difference 4°C). This can be explained partly by larger grid elements in the simulation, necessitated by the larger dimensions of the problem. Furthermore, the injection and extraction data was quite sparse, consisting of only one measurement for some months. Additional changes in the extraction temperature may also be a result of the precipitation and the infiltration of rain water into the aquifer, which was not accounted for in the simulation.

In spite of temperature averaging, the energy balance compared fairly well, the measured and simulated energy recovery ratios being 68.6% and 64.4%, respectively, corresponding to a change of only 0.3°C in the average extraction temperature. As to temperature contours (Publication III) the same trend as in the hot water experiment can be observed: the simulated contours reach further than the measured ones.

The results of a sensitive analysis performed on the most important simulation parameters are included in Table 6.2. The permeability, heat capacity and the vertical location of the well screens are the most sensitive parameters.

![Diagram](XBL849-9964)
6.4 The SPEOS experiment

SPEOS (Stocakge Pilote d'Energie par un Ouvrage Souterain) (Doughty and Tsang, 1985; Stultz, 1985) was an aquifer experiment conducted by the Lausanne University of Technology and the Lausanne University. It was also a part of the energy storage programme of International Energy Agency (IEA). The specific properties of this experiment include anisotropic as well as layered permeability. As shown in Fig. 6.9, the aquifer consists vertically of two water conducting layers, separated by a clay layer.

Also the well arrangements are different, with horizontal wells instead of vertical used to charge and discharge the heat. During the storage phase, water is extracted from the lower layer, heated in heat exchangers and the returned to the upper layer. During discharge, the flow is reversed.

The physical properties of the aquifer are shown in table 6.4. The natural groundwater flow rate at the site was about 35 m/year and the temperature 12°C. Hydraulic gradient was 0.68%.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>unsaturated zone</td>
<td>horizontal permeability</td>
<td>$k_h = 1.26 \cdot 10^{-14} \text{ m}^2$</td>
</tr>
<tr>
<td></td>
<td>vertical permeability</td>
<td>$k_v = 1.26 \cdot 10^{-15} \text{ m}^2$</td>
</tr>
<tr>
<td></td>
<td>thermal conductivity</td>
<td>$\lambda = 2.1 \text{ W/m}^2\text{K}$</td>
</tr>
<tr>
<td></td>
<td>heat capacity</td>
<td>$\rho C = 2 \cdot 10^6 \text{ J/m}^3\text{K}$</td>
</tr>
<tr>
<td>upper aquifer</td>
<td>horizontal permeability</td>
<td>$k_h = 8.16 \cdot 10^{-12} \text{ m}^2$</td>
</tr>
<tr>
<td></td>
<td>vertical permeability</td>
<td>$k_v = 1.27 \cdot 10^{-13} \text{ m}^2$</td>
</tr>
<tr>
<td></td>
<td>thermal conductivity</td>
<td>$\lambda = 2.5 \text{ W/m}^2\text{K}$</td>
</tr>
<tr>
<td></td>
<td>heat capacity</td>
<td>$\rho C = 3 \cdot 10^6 \text{ J/m}^3\text{K}$</td>
</tr>
<tr>
<td>clay zone</td>
<td>horizontal permeability</td>
<td>$k_h = 3.77 \cdot 10^{-12} \text{ m}^2$</td>
</tr>
<tr>
<td></td>
<td>vertical permeability</td>
<td>$k_v = 6.41 \cdot 10^{-15} \text{ m}^2$</td>
</tr>
<tr>
<td></td>
<td>thermal conductivity</td>
<td>$\lambda = 2.1 \text{ W/m}^2\text{K}$</td>
</tr>
<tr>
<td></td>
<td>heat capacity</td>
<td>$\rho C = 2.5 \cdot 10^6 \text{ J/m}^3\text{K}$</td>
</tr>
<tr>
<td>upper aquifer</td>
<td>horizontal permeability</td>
<td>$k_h = 8.16 \cdot 10^{-12} \text{ m}^2$</td>
</tr>
<tr>
<td></td>
<td>vertical permeability</td>
<td>$k_v = 1.27 \cdot 10^{-12} \text{ m}^2$</td>
</tr>
<tr>
<td></td>
<td>thermal conductivity</td>
<td>$\lambda = 2.5 \text{ W/m}^2\text{K}$</td>
</tr>
<tr>
<td></td>
<td>heat capacity</td>
<td>$\rho C = 2.5 \cdot 10^6 \text{ J/m}^3\text{K}$</td>
</tr>
</tbody>
</table>
During 1982-1984, two experiments were conducted. The charge and discharge periods were 137 and 77 days in the first cycle, and 177 and 113 days in the second cycle, respectively. The average temperatures of the injected water were 59.3°C and 69.5°C. The amount of discharged water was about 1.2 times that of charged in both cycles. The resulting energy recovery ratios were

\[ \eta_{1, \text{cycle}} = \frac{323 \text{ MWh}}{783 \text{ MWh}} \approx 0.41 \quad \text{and} \quad \eta_{2, \text{cycle}} = \frac{542 \text{ MWh}}{1306 \text{ MWh}} \approx 0.42 \]

In the simulation, a grid with horizontal dimensions of 22 x 24 points with 20

Fig. 6.10: Measured and simulated extraction temperature in SPEOS.
Table 6.5: Sensitivity analysis for SPEOS.

<table>
<thead>
<tr>
<th>property</th>
<th>change</th>
<th>( \eta, % ) (cycle 1)</th>
<th>( \eta, % ) (cycle 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(reference)</td>
<td>-</td>
<td>44.0</td>
<td>45.2</td>
</tr>
<tr>
<td>permeability</td>
<td>+20%</td>
<td>41.7</td>
<td>42.2</td>
</tr>
<tr>
<td>hydraulic gradient</td>
<td>+20%</td>
<td>41.7</td>
<td>42.2</td>
</tr>
<tr>
<td>aq. thermal conductivity</td>
<td>+20%</td>
<td>41.3</td>
<td>42.6</td>
</tr>
<tr>
<td>aq. heat capacity</td>
<td>+20%</td>
<td>44.9</td>
<td>47.1</td>
</tr>
<tr>
<td>heat loss to amb. air</td>
<td>+20%</td>
<td>43.9</td>
<td>45.1</td>
</tr>
</tbody>
</table>

vertical layers was set up. The grid spacing was 3.7 m in horizontal and 1.4 m in vertical direction. The spacings were chosen so that well arrangement could be simulated as accurately as possible. The injection temperature as well flow rate were assumed to have a constant value, with the exception of three pauses in the second experiment.

The simulated and measured extraction temperatures as a function of time are shown in Fig. 6.10. For the first cycle, the fit in extraction temperature is good, with the final temperature difference being 2.3°C. The sudden jump in the temperature curves was caused by the closing of two extraction pipes. For the second cycle, the fit is not as good as in the first cycle. One reason for this is that during the extraction, two vertical pipes connecting the two groundwater layers were installed in the ground. Due to insufficient information, it could not be accounted for in the simulation. Furthermore, the initial state of the aquifer in the beginning of the experiment was not very well known.

The simulated energy recovery ratios for the two cycles were 44% and 45%, respectively. Comparing to changes caused parameter uncertainties shown in table 5.3, this is a good fit.
7. APPLICATIONS

7.1 Ground as a heat source for a heat pump

(Publication V)

There already exists ample experience of the use of ground as a heat source e.g. for heat pumps (Sanner and Lehmann, 1994). The heat content of the ground is continuously refreshed by solar radiation and other heat transfer processes from the atmosphere. The ground heat is thus utilisable as such, although improved performance can be achieved by actively storing heat and thus regenerating the heat content of the ground.

The structures needed are fairly simple, consisting usually mainly of a heat pump connected to a network of pipes that is buried in the ground. The effect on scenery and visible environment is thus minimal, as most of the system is hidden beneath the earth surface. The ground above the pipes is, with some limitations, usable for e.g. agriculture and building construction.

The most prominent limitation of the ground heat extraction systems is the decrease of ground temperature, which not only limits the available energy but may also cause environmental problems. Although groundwater enhances the performance of a ground heat extraction system through its good heat transfer properties, the freezing of water in the ground may cause problems in the form of frost heave.

To study the performance of a ground heat extraction system in the absence or presence of groundwater, THETA was used to simulate heat extraction in various conditions. Because of the multitude of affecting parameters, however, only those considered most important could be considered. The heat extraction was simulated by a constant extraction power, which was turned on or off as specified by system control. The effect of artificial recharge, or storing heat in the ground to compensate the extraction, was also studied.

In the simulations, it was found that groundwater flow rate and other geological parameters and limitations (minimum allowable ground temperature) have a profound effect on the behaviour of a ground heat extraction system. For instance, in the base case with no natural groundwater flow, a no-freeze limitation set on the minimum temperature in the ground restricted the amount of recoverable heat to 10% of the maximum value obtainable. With the introduction of natural groundwater flow, the discharge efficiency increased to 27% - 100%, depending
Fig. 7.1: Ground temperature at extraction location with (a) zero and (b) non-zero groundwater flow.

on the flow rate The increase was due to natural regeneration of the ground heat by groundwater flow.

The enhancement in heat transfer provided by groundwater is clearly illustrated by Fig. 7.1, which shows the ground temperature at the heat extraction location.
The cyclic behaviour of the extraction power is due to the minimum temperature limitation. As can be seen from the figure, in the presence of groundwater flow the number of cycles is increased, leading to a better energy recovery. With high enough groundwater flow rate, the cyclic behaviour was found to disappear leading to a constant extraction, which is ideal e.g. for a heat pump.

It was also found that in the presence of groundwater, the cold pulse resulting from the cooling of the ground moves downstream, being hundreds of meters even with the modest groundwater flow rates considered in the study (natural groundwater flow rate 35-70 m/year). With the high flow rates present in Nordic esker aquifers disturbance distances of few kilometres can be expected.

The geometry of the extraction configuration also has a profound effect on the extraction system performance. Not only the vertical location of the heat exchangers, but in the case of artificial recharge, also the horizontal location of the recharge and extraction wells was found to be an important design parameter.

7.2 Thermal energy storage systems

(Publication IV)

In design the of an energy system based on thermal energy storage in an aquifer, the aquifer geohydrology and storage temperature levels must be carefully considered. Temperature levels must be adjusted to the desired load temperature by the use of heat pumps if necessary. The groundwater flow rate, on the other hand, is the determining factor for the well design. With moving groundwater, charge and discharge wells must be located so that the stored energy reaches the recovery area at a right time. With a heat pump, evaporator input and discharge wells have to be placed far enough from each other to prevent the cold pulse from reaching evaporator input.

The task of designing an energy system with thermal storage was approached by simulation model AQSYST, which is a special version of the program THETA. In AQSYST, the total system to be simulated is formed by combining subsystems which are simulated separately. A special connection matrix formalism provides a way to connect these subsystems in a desired way. One of these subsystems is the aquifer storage which is simulated by THETA.

The simulations presented in Publication IV form a part of a larger study conducted earlier (Kangas and Lund, 1988). The basic system configuration, as depicted in Fig. 4.5, included a low to high temperature heat source and a heat load, the latter consisting of the space heating and hot water demand of a number
of residential houses in a district heating system. A heat pump was used to increase the temperature level of the heat obtained from the storage, if necessary.

The simulations showed that there exists an intimate link between the type of heat load and the demands set on the geological characteristics of the aquifer. A heating system with high temperature storage requires an aquifer with a low groundwater flow rate. Otherwise, the processes associated with the transfer of stored heat or heat losses cause a considerable loss in temperature level, or energy quality. This results in inefficient storage utilization as well as a low non-purchased fraction of energy (F), defined as:

\[
F = 1 - \frac{Q_{aux}}{Q_{load}},
\]

where \(Q_{load}\) is the heat load and \(Q_{aux}\) the auxiliary energy demand (boiler, heat pump compressor etc.).

Two extreme cases were considered in detail in the study: natural solar heat (low temperature) storage in a high flow aquifer and a high temperature storage in a low flow aquifer. As to non-purchased factor of energy, both systems were found to be promising, with \(F = 49\%\) and \(F = 62\\%), respectively. The steady state with steady yearly average storage performance was in both cases reached in four years.

Figure 7.2 shows a qualitative assessment of the aquifer heat storage potential for different storage temperature requirements, depicted on the basis of the simulations in this and in an earlier study (Kangas and Lund, 1988). With storage temperature as the storage classification criterion, low temperature storage can be seen to be potential in all kind of aquifers, whereas high temperature storage is efficient only in low flow aquifers.

The groundwater flow rate sets also requirements on the well geometry of the storage system. With low groundwater flow, the injection and recovery well must be located close to each other, whereas with high flow the wells must be located far enough to allow the stored heat flow with groundwater to the recovery well during the specified storage time.
7.3 Thermohydraulic analysis of nuclear waste disposal in rock

(Publications VI and VII)

The present plans of the final disposal of radioactive spent fuel from nuclear power stations in Finland are based on the Swedish KBS-3 concept (Peltonen, 1987; Bergman et al., 1984). Spent fuel will first be encapsulated in copper canisters which are then placed into holes drilled in the floors of horizontal tunnels at the depth of 500 meters in crystalline bedrock (Peltonen, 1987; Rasilainen et al., 1993; Vieno, 1994). A multiple barrier system, based on both engineered and natural barriers is designed to isolate the waste from the environment as long as the radioactivity is harmful.

Groundwater provides the most important pathway for radionuclides up to the biosphere. For safety analyses, it is thus essential to be able to calculate the groundwater flow field near the repository. In order to minimize the risks associated with waste disposal, a geological environment where the groundwater flow is at a minimum is desirable.
Fig 7.3: Two-dimensional groundwater flow patterns generated by radiogenic heat production with (a) constant permeability, (b) permeability decreasing with depth, and (c) fractured rock. The two areas, to the left and right of the vertical line at x=10 km, had heat production densities and thermal conductivities of $\lambda_1 = 5 \text{ } \mu \text{W/m}^3$, $\lambda_1 = 3 \text{ W/Km}$ and $\lambda_1 = 1 \text{ } \mu \text{W/m}^3$, $\lambda_1 = 2.5 \text{ W/Km}$, respectively.
The groundwater flow in bedrock is affected not only by topological conditions but also by possible heat generation in the ground (Kukkonen, 1989). The heat generation process can be either natural, resulting from the radioactive decay of the natural elements within the bedrock, or artificial, being caused by the disposed waste itself.

In the first phase of the study (Publication VI), the effect of differences in natural radiogenic heat production on groundwater flow patterns in the bedrock was studied by two-dimensional simulations. The main aim of the simulations was to widen the approach of an earlier study to include the temperature dependence of water viscosity as well as vertical changes in permeability and fracture zones. The effect of a regional hydraulic gradient was also studied.

The simulation domain consisted of two adjacent regions with different heat production rates and thermal conductivities. The resulting flow patterns corresponded with few exceptions qualitatively to the earlier results obtained with a simpler model and more restricting assumptions. Depending on the permeability of the bedrock, a pattern consisting of one, two or more convection cells was formed.

Quantitatively, however, there were significant differences. The inclusion of temperature dependent viscosity increased the flow rates to 2-5-fold. In case of vertically changing permeability and fracture zones the changes were even greater, high flow rates being higher, as was expected, in the regions with higher permeability. Figure 7.3 shows as an example 2-dimensional flow patterns for three cases differing only by permeability distribution. With heterogeneous permeability, a clear concentration of flows near the surface and in the fractures can be observed.

When a regional hydraulic gradient was included, it was observed that even with small gradients, the groundwater flows generated by differences in radiogenic heat generation were insignificant as compared to the flows resulting from regional gradients.

In the second phase (Publication VII), a 3-dimensional thermohydraulic analysis was performed on an planned waste disposal site in northern Finland. The aim of the study was to assess the effect of fractures and increased temperatures due to waste generated heat on groundwater flow patterns. Flow field both in the vicinity and far from the repository site was considered. The duration and dimensions of the temperature perturbation in rock were of particular interest.
Figure 7.4 shows groundwater table at the simulated site, which also corresponds the form of the ground surface. Only the flows below general ground level (represented by the level $z=0$ in Fig 7.4) were considered. The higher groundwater level in the middle was represented by a pressure head and proper boundary conditions.

In addition to fracture zones, permeability decreasing with depth was included in the simulation. However, based on the findings of the previous phase about the dominating effect of hydraulic gradient, radiogenic heat production was not considered.

As in the previous phase, the groundwater flow was found to be very heavily concentrated in the fractures, the maximum flow rates (Darcy flow) being about 2 metres/year, or 30000-fold compared to the flows (0.06 mm/year) in the unfractured rock at the planned disposal depth of 500 metres. It was also found that due these very small flow rates, heat transfer by convection is insignificant in the vicinity of the repository site.

The effect of waste repository heat generation was then assessed by adding a power source corresponding to the heat generated by 1260 MgU of spent nuclear fuel with a burn-up of 35 MWd/kgU and a cooling time of 10 years. The Darcy velocity near the repository was observed to increase to about four-fold, the direction of the flow at the same time changing toward vertical because of buoyancy effects. At some fracture locations, even 60-fold increase was observed.

The effect of the heat generation can most clearly be seen from the piezometric head contours, shown in Figure 7.5 before (a) and 70 years after the disposal (b).
Fig. 7.5: Piezometric head contours in a vertical cross section (a) before and (b) 70 years after the disposal. Thick lines represent fracture zones.

The numbers shown in the figure give the value of the head in metres above sea level. 70 years was chosen for the second datum because it is the time after which maximum temperature is reached in the repository.

It was found that the changes in flow field in the vicinity of the repository are clear during the first 5000 years. The temperature changes concentrate into a volume with a diameter of about 800-1000 m. In case of early release of radioactive waste, the temperature effects may speed up the transport of radioactive material not only by increasing the flow rate but also by changing the flow directions, which may cause the flow to reach more permeable areas resulting in faster transport paths. Temperature effects should thus be taken into account when choosing the location of repository relative to the existing fracture zones.
7.4 Solute transport analysis

*Publication VIII*

Although THETA has been mainly developed for thermal analyses, routines for the analysis of solute transport in porous media are also included in it to enable more comprehensive analyses.

In this study, simulation model THETA has been described with emphasis on environmental applications and solute transport. A sample application with the transport of a soluble non-radioactive solute in groundwater was simulated. This kind of situation can arise e.g. as a result of an environmental accident.

In case of an environmental accident consisting of a spill of some unwanted material into the aquifer, one possible remedy is to inject pure water and thus dilute the spilled material in the ground. Figure 7.6 illustrates the effect of fresh water injected into the aquifer after the spill. The solute temperature was 7°C, and fresh water injection started immediately after the solute infiltration. Two cases with fresh water temperatures 70°C and 7°C were simulated. With lower temperature, the dilution of solute concentrations takes place faster. With higher temperatures, buoyancy causes upward flows leaving concentration "pockets" near the bottom of the aquifer.

Fig. 7.6 : Concentration contours in a vertical cross section with fresh water injection (7°C (upper) and 70°C (lower)) following the solute injection (conc. 100 units, 7°C).
8 DISCUSSION AND CONCLUSIONS

8.1 Simulation model THETA

The aim of this thesis was to develop means for analyzing transport processes in porous media. The stress on the studies was on energy-related applications, mostly in the transfer of heat in the ground and groundwater. However, not only the direct utilization of groundwater, such as for thermal energy storage, but also the impact of this utilization on groundwater quality was of concern. Thus, chemical species transport was given some consideration.

To make the reaching of this goal possible, an accurate knowledge and careful evaluation of the transport processes in porous media, of which aquifers are one representative, was needed. The associated physical processes are in general very complicated, and, for example in case of an accurate description of buoyancy flows, necessitate a fully 3-dimensional treatment. Analytical methods are seldom enough, and numerical models must be used. In case of aquifers, the situation is further complicated by the site specific nature of the problem: the changes in parameters values can be several orders of magnitude, complicating the approximations needed in an analytical approach to a real problem.

As the result of this thesis, a design and evaluation tool THETA for various energy related porous medium applications has been developed. The intended main use of the model is the simulation of water in ground (aquifers), but with some restrictions the model is also applicable to more general porous medium flow applications. The main emphasis in the thesis has been on novel utilization of known numerical methods and the development of a model capable of simulating various porous media applications, and not the numerical methods themselves.

The model simulates the coupled transport of fluid, heat and solute in porous media. The thermal part of the model has been validated using measured data from three different field experiment, chosen to represent a wide variety of physical parameters and system configurations.

THETA is mainly intended to be used on a microcomputer, for which a specific graphical user interface has been developed. However, excluding the user interface, the model can very easily be transported to various
computing platforms ranging from UNIX workstations to main frame or even super computers.

The main limitations of the model are its confinement to the saturated porous medium flows only and the restrictions and simplifications in the solute transport code. In the present version of THETA, for example, the infiltration from the ground surface to the groundwater can be accounted only by proper boundary conditions at the upper edge of the saturated zone. A future enhancement of the model would thus be routines for calculating the transport also in the unsaturated zone. The model is also not capable to accurately reflect more complicated geometries. As to solute transport, further improvements include methods to better account for numerical dispersion as well as addition of reactive transport model.

8.2 Applications of THETA

In the thesis, THETA has also been applied to various studies ranging from thermal energy storage system evaluations to nuclear waste disposal simulations (Publications IV-VIII; Eerikäinen et al., 1992). A model comparison has also been made (Kangas and Peltola, 1989; Peltola, 1989). In the applications, the model has proven to be a versatile tool and easily applicable in various situations.

The main result of the study of aquifer as a heat storage in a district heating system was the classification of aquifers that are potential as an energy storage in different heating systems. The aquifer classification was based on their geogydraulic properties, mainly on the groundwater flow rate. It was found that the so called esker aquifers, characterized by a high groundwater flow rates and which are common in Nordic conditions, are suitable only for low temperature storage. Thermal storage based on a high storage temperature necessitates an aquifer with a very slowly flowing, or ideally stagnant, groundwater.

When the ground itself is used as a heat source for a ground coupled heat pump, it was found the environment sets strict limits to the utilizable heat. If freezing is to be avoided, the energy output of the heat pump may be severely limited by the necessity to repeatedly turn off the heat extraction. The simulations showed that in the presence of groundwater flow, the performance of the heat extraction system is improved, as the groundwater transfers new heat to the extraction area, thus diminishing the need to shut down the heat extraction because of temperature decrease.
The main aim of the nuclear waste disposal studies performed in this thesis was to evaluate the effect of temperature changes on the groundwater flow pattern in the vicinity of a waste disposal site. At the time of the studies, the effect of temperature changes had not been thoroughly accounted for in the evaluations done on the safety of nuclear waste disposal in the rock. The simulations performed with THETA revealed that although the flow rates around the disposal site are small compared to the flows in the fractures surrounding the repository, they can be increased to five fold because of the heat generated by the radioactive decay in the disposed waste. A significant change in the groundwater flow revealed by the 3-dimensional simulation with THETA was a change in flow directions caused by buoyancy flows.

As to the solute transport routines included in THETA, it was found that as such they have some limitations which prohibit their use in comprehensive and accurate solute transport calculations. Notably, these include numerical dispersion inherent in the transport code. They do, however, give valuable insight into the combined effects of heat and solute transport.
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