Heat transfer processes in the upper crust: influence of structure, fluid flow, and palaeoclimate

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Far better an approximate answer to the right question, which is often vague, than an exact answer to the wrong question, which can always be made precise.

John W. Tukey, 1962
ABSTRACT

Numerical models constrained by geological and geophysical data form the basis of understanding the thermal regime of the Earth’s crust. This dissertation focuses on modelling heat transport in the upper crust, studying the relative contributions of different processes to the specific heat flow distribution. Its vertical variation is a well known fact, caused by different processes such as changes in surface temperature, fluid flow, and heterogeneity. In particular, the first one can provide valuable information. Since the subsurface temperatures are directly related to past temperatures, their inversion into ground surface temperature histories are the only method available in palaeoclimatology to construct palaeotemperatures without using indirect proxy methods. Furthermore, a general better understanding of the processes affecting the thermal regime of the upper crust is needed for better downward continuation of thermal data, which is important for considerations about the thermal evolution of the lithosphere.

A large geothermal data set from the Kola peninsula is processed and described in detail in order to prepare it for a numerical case study simulating heat transport processes in the Kola super-deep hole area. The data set includes 3400 measurements of thermal conductivity on 1375 samples from 21 boreholes with a depth up to 1.6 km and 36 temperature logs. The modelling involves 3-D forward simulation of both conductive and advective heat and mass transfer, and 1-dimensional inverse modelling for the palaeoclimatic ground temperature changes in the study area. Steady-state and transient 3-D models as well as the inverse modelling allow to estimate and quantify systematically the influence of fluid flow, spatial heterogeneity of thermal properties of rock, and palaeoclimate on the subsurface temperature field. Being aware that the information on permeability is sparse, the modelling results suggest that advection has a major influence on the vertical specific heat flow distribution. This is confirmed by inversion results which show higher temperatures during the last glacial maximum than in other areas, indicating an insulating effect of a persisting ice cover. However, forward modelling demonstrates that transient changes in surface temperature cannot be totally neglected, because their influence may reach more than half of the magnitude of the advective effects, depending on the assumed permeability and the particular climate model.

The northern location of the study area required to implement latent heat effects by thawing and freezing of pore water in the numerical forward and inverse codes. So far, most geothermal investigations on past ground temperature histories in northern areas and during cold climatic episodes have not taken into account these effects. Depending on different parameters, such as the freezing period, surface temperature, and porosity, the influence on modelling results can be substantial. Since the modelling results show that latent heat effects can be neglected in the low porosity crystalline environment of the Kola area, the impact of freezing processes is shown for an example in the East European Platform. Whereas the inversions including freezing effects yield a postglacial warming of about 18 K, the neglect of latent heat effects would overestimate this result by some 6 K.

This result is generalised by a study about the freezing and thawing processes in subsurface inverse modelling for a wide range of the above-named parameters. This allows to provide a more universal character-
isation of the influence of latent heat effects on past temperature reconstructions by inversion. For possible corrections of existing ground surface temperature histories derived from borehole measurements, parametric relationships are developed which describe quantitatively the magnitude of these effects in terms of porosity, basal specific heat flow, present-day and past ground surface temperature history. Since a large number of synthetic model runs were required, it was necessary to modify the applied Tikhonov inversion method. In this approach, a regularisation parameter has to be determined, representing a trade-off between data fit and model smoothness. This is achieved by the general cross validation method which makes the inversion for past temperatures faster, more automatic, and more objective. It is employed in a synthetic example, as well case studies from the Kola ultra-deep drilling site and another borehole from northeastern Poland. Although the convergence of the inversion iterations are rather different in these three cases, a satisfactory final result was obtained in each of them. Thus, this novel approach in the field of palaeotemperature inversions contributes to the current efforts to optimise the inversion methods for palaeotemperature reconstructions.

Parts of this work have been published, submitted, or are in preparation for publication in the following papers:


ZUSAMMENFASSUNG


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1. INTRODUCTION

Understanding the factors which control the Earth’s thermal regime is essential when using thermal data to determine the temperature distribution and fluid flow rates in the subsurface, as well as the variation of the Earth’s temperature in the historic and geologic past. Data is derived from borehole measurements and geological and geophysical observations, such as seismic soundings. Since this information is generally sparse, conclusions drawn from modelling of physical processes need to be thoroughly discussed in terms of predictions and uncertainties. The next section provides a brief introduction into thermophysical processes, being the basis for subsequent modelling and deeper discussions presented in the following chapters. Thereafter, the modelling techniques are presented and the last two sections of this chapter describe the current state of research in this field and summarise the aims of this dissertation.

1.1 Heat transfer processes

Thermal energy in the subsurface is transferred from the warm to the colder levels. Heat is transferred by conduction, convection, and radiation, all of which may occur separately or in combination. In steady-state conditions thermal conductivity is important next to the temperature difference. In transient heat flow problems, thermal diffusivity which is the ratio of thermal conductivity and the product of density and specific heat capacity takes the place of thermal conductivity. Both of these properties are functions of temperature. Convective heat transfer is controlled by two different driving forces for fluid flow: (1) buoyancy produced by density differences due to heat expansion of viscous rock or pore fluid (free convection in the mantle or in an aquifer) and (2) pressure gradients due to topographically controlled variations in the groundwater table (advection or forced convection) yield moving fluids. Permeability is the dominating parameter controlling flow magnitudes. Radiative heat transfer in contrast depends on temperature according to the Stefan-Boltzmann law. In geological media, opacity is the critical property of the rocks controlling the efficiency of radiation. Since this work addresses the upper crust where radiation as a heat transport mechanism can be neglected, the focus lies on heat conduction and convection. In the following, the basic principles of these mechanisms are illustrated.

1.1.1 Heat conduction

Fourier’s first law, experimentally derived, describes heat conduction which is for the one dimensional case

\[ Q = -F \frac{\lambda(T_2 - T_1)}{h}, \]

(1.1)

here \( Q \) is the heat flow (W), \( \lambda \) is thermal conductivity (W m\(^{-1}\) K\(^{-1}\)), \( T_2 - T_1 \) is the temperature difference (K) between two planes, parallel boundary surfaces, \( F \) is the surface area (m\(^2\)), and \( h \) is the thickness of
the wall (m). The specific heat flow \( q \) (W m\(^{-2}\)) is

\[
q = -\lambda \frac{dT}{dh} \approx \frac{Q}{F}.
\]

(1.2)

This forms the basic equation which has to be used to determine geothermal specific heat flow in boreholes by temperature measurements at different depths and laboratory measurements of thermal conductivity on rock samples. Expanding the problem to three dimensions yields

\[
q = -\lambda \nabla T,
\]

(1.3)

where \( q \) and temperature gradient are vectors and \( \lambda \) is the thermal conductivity tensor.

On the one hand, the net heating or cooling of the control volume \( dV = dx \cdot dy \cdot dz \) by thermal energy flowing through the volume per unit time is defined by

\[
P_{\text{flow}} = -\left( \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} \right) dV,
\]

(1.4)

where \( P \) is power (W). The vertical heat flow \( dq_z \) through the plate \( dx \cdot dy \) is \( \frac{\partial q_z}{\partial z} dV \) (\( dq_x \) and \( dq_y \) correspondingly). On the other hand, thermal energy stored per unit time in the control volume \( dV \) is

\[
P_{\text{stored}} = \rho c_p dV \frac{\partial T}{\partial t}.
\]

(1.5)

Here, \( \rho \) is the density (kg m\(^{-3}\)), \( c_p \) is specific heat capacity (J kg\(^{-1}\) K\(^{-1}\)), \( dV \) is the volume (m\(^3\)), and \( \frac{\partial T}{\partial t} \) is the temperature change per unit time \( t \) (s).

Combining equations (1.4) and (1.5) yields Fourier’s second equation

\[
-\nabla \cdot q = \rho c_p \frac{\partial T}{\partial t}.
\]

(1.6)

Using (1.3) the expression in (1.6) becomes

\[
\lambda \triangle T = \rho c_p \frac{\partial T}{\partial t},
\]

(1.7)

and when assuming isotropic rock material in terms of thermal conductivity (\( \lambda_x = \lambda_y = \lambda_z = \lambda \)):

\[
\frac{\partial T}{\partial t} = \kappa \triangle T,
\]

(1.8)

with \( \kappa = \lambda/\rho c_p \) being thermal diffusivity, which governs the heat transport equation (1.8). If there is internal heat generation in the medium, an additional term appears:

\[
\frac{\partial T}{\partial t} = \kappa \triangle T + \frac{H}{\rho c},
\]

(1.9)

where \( H \) is the heat generation rate (W m\(^{-3}\)). Heat generation of rocks is mainly caused by the decay of radioactive isotopes, but also possibly by mineral reactions during diagenesis and metamorphism. The radiogenic heat generation rate in rocks depends on the abundances of the elements uranium, thorium and potassium. Only these naturally radioactive isotopes contribute appreciably to heat generation. According
to Rybach (1988), heat generation $H$ is:

$$H = 10^{-5} \cdot \rho \cdot (9.52c_U + 2.56c_{Th} + 3.48c_K), \quad (in \ \mu W m^{-3}).$$

(1.10)

Here, $c_U$, $c_{Th}$ and $c_K$ are the abundances of uranium, and thorium (weight ppm), and potassium (weight %).

Equation (1.9) forms the basis for studying conductive geothermal problems. The most common ones are those where the equation is solved as a boundary value problem with known surface temperature and mantle heat flow. Carslaw and Jaeger (1959) give analytical solutions for a variety of boundary conditions. However, all these analytical solutions require a homogenous or layered model with constant thermophysical properties. As an example, equation (1.11) shows the analytical solution for the special case of a semi-infinite, homogenous solid, extending from $x = 0$ to infinity in the positive $x$ direction, whose initial (at time $t = 0$) temperature is $T_0$ and the surface $x = 0$ is kept at zero degrees:

$$T(t) = T_0 \text{ erf} \left( \frac{x}{2\sqrt{\kappa t}} \right),$$

(1.11)

where $\text{erf}$ is the error function. Here, the governing character of thermal diffusivity $\kappa$ becomes obvious. However, in order to resolve from the limitations connected with the analytical solutions, in this work, equation (1.9) and related differential equations are solved numerically, which allows to include nonlinear variations of the governing thermophysical properties.

**Thermal conductivity**

Thermal conductivity of the rocks in the Earth’s crust can vary within a large interval, from less than 1 W m$^{-1}$ K$^{-1}$ to about 8 W m$^{-1}$ K$^{-1}$, with extremes of graphite or talc bearing rocks often reaching 10 W m$^{-1}$ K$^{-1}$ – 12 W m$^{-1}$ K$^{-1}$ (e.g. Clauser, 2006). It shows a non linear temperature and pressure dependence. A typical equation for temperature dependence of lattice (phonon) thermal conductivity is

$$\lambda = \frac{1}{aT + b}.$$  

(1.12)

where $a$ (W$^{-1}$ m) and $b$ (W$^{-1}$ K m) are constants related to phonon scattering (Schatz and Simmons, 1972). In rocks, radiative heat transfer becomes relevant only at temperatures above about 1000 K which is far above the temperatures studied in this work.

Data from the literature indicates that common rock types show more or less similar temperature dependent behaviour, although results from individual minerals can be very different and strongly influenced by anisotropy (e.g. Clauser and Huenges, 1995). In general, thermal conductivity of quartz-rich rocks decreases more rapidly with temperature than that of quartz–poor rocks. For instance, Seipold (1998) compiled available data of crystalline rocks regarding temperature dependence and fitted them to equation 1.12. However, since in this work there is a large data set on thermal conductivity available, it is used to fit equation 1.12 and in subsequent modelling rather than other relationships presented in the literature (see section 2.2.1).
Heat capacity

Because of certain self-compensating factors, thermal capacity $\rho c_P$ at ambient temperature varies within $\pm 20\%$ of $2.3 \times 10^6$ J m$^{-3}$ K$^{-1}$ for the great majority of minerals and impervious rocks (Beck 1988). This relationship is verified in this work. Temperature dependence of thermal capacity (or volumetric heat capacity) $\rho c_P$ is dominated by that of specific heat capacity, since the thermal volumetric expansion coefficient of crystalline rocks is very small, in the order of $\mu K^{-1}$. The temperature dependence of the specific heat capacity $c_P$ of rocks can be described by a second-order polynomial (Kelley 1960):

$$c_P = \sum_{i=0}^{2} A_i T^i.$$ (1.13)

The regression using the data in this work is discussed in section 2.2.4.

Thermal diffusivity

Since thermal diffusivity $\kappa$ controls the time dependent temperature change (equation 1.8), it is important to characterise this parameter properly. In particular, the temperature dependence of thermal conductivity and thermal capacity are important for subsurface heat transport, because their opposite behaviour result in a significant temperature dependence of thermal diffusivity. This is shown in section 2.2.4, where a deeper discussion and an application to data is presented.

1.1.2 Heat advection

Fluid flow through the rock matrix contributes to heat transfer. It is

$$q = \nabla \cdot (\rho_f c_f v_D T).$$ (1.14)

Here, $q$ is specific heat flow due to convection, $\rho_f$ and $c_f$ are density and specific heat capacity of the fluid. $v_D$ is the Darcy velocity (specific discharge), defined as $v_D = v_a \phi$, with the particle velocity $v_a$, combining the average linear velocity of a water molecule and $\phi$ the porosity of the matrix. Darcy’s original experimentally derived law (published in 1856) describes the relationship between $v_D$ and the gradient in hydraulic head $h$ (dimensionless) in three dimensions

$$v_D = -K \nabla h,$$ (1.15)

where the hydraulic conductivity $K$ (m s$^{-1}$) is the constant of proportionality. It is itself a combination of fluid and solid properties, proportional to the specific weight of the fluid $\rho_f g$, inversely proportional to the dynamic viscosity of the fluid $\mu_f$, and proportional to a property of the solid medium, $k$, which is called permeability:

$$K = \frac{k \rho_f g}{\mu_f}.$$ (1.16)

Permeability is the most crucial hydrologic parameter (Ingebritsen et al. 2006). In common geologic media it can vary by 16 orders of magnitude, from as low as $10^{-23}$ m$^2$ in intact crystalline rocks to as high as $10^{-7}$ m$^2$ in well-sorted gravels.
The convective part completes the heat transport equation (1.9) which after re-arranging is:

\[ \nabla \cdot (\lambda \nabla T - \rho_f c_f T \mathbf{v_D}) + H = \frac{\partial T}{\partial t} (\phi \rho_f c_f + (1 - \phi) \rho_m c_m) \] (1.17a)

\[ \nabla \cdot (\lambda \nabla T - \rho_f c_f T \mathbf{v_D}) + H = 0. \] (1.17b)

Equation (1.17a) is the transient heat transport equation, whereas equation (1.17b) describes the steady state case. The first term on the left specifies the transport of heat by conduction with the thermal conductivity tensor \( \lambda \); the second one specifies advection by motion of pore fluid with Darcy velocity \( \mathbf{v_D} \). In (1.17a), the subscripts \( f \) and \( m \) account for the two-phase mixture between solid rock (\( m \)) and fluid-filled pore space (\( f \)) in a saturated medium. This mixture is characterised by porosity \( \phi \). Both, thermal capacity \( \rho c \) and thermal conductivity are functions of temperature and pressure. For thermal capacity, as a scalar, a simple arithmetic mixing applies (often referred to as Kopp’s law). In contrast, mixing laws for determining thermal conductivity require a deeper discussion (see e.g. Clauer 2006). From equation (1.17) it is obvious that hydrologic flow may seriously affect specific heat flow determined from borehole measurements.

1.1.3 Palaeoclimate as a transient boundary condition

When studying heat transfer in the Earth’s upper crust, the upper boundary condition of equation (1.17) is constrained by the local climatic conditions. Variability of this conditions induces a transient signal which diffuses into the subsurface. Thus, ground temperatures comprise an archive of past climate signals. Reconstructing those is of major interest since one of the most important components of climatic change is the variation of temperature at the Earth’s surface. The distribution of ground temperature is a linear function of depth in an idealised homogeneous crust with a constant surface temperature. Decreasing temperatures at the surface will cool down the rocks near to the surface, resulting in a larger thermal gradient at shallow depth and temperature profiles with curvature like the one shown in light grey in figure 1.1. An increasing warming, on the other hand, is responsible for a temperature profile with smaller thermal gradients at shallow depth like the one shown in dark grey in figure 1.1. If the surface temperature oscillates with time, this results in corresponding oscillations of the ground temperature. The magnitude of the departure of ground temperature from its undisturbed steady state is related to the amplitude of the surface temperature variation. The depth to which these disturbances can be measured is related to the timing of the original temperature change at the surface. Due to the low thermal diffusivity, changes in ground surface temperature propagate downward slowly. Accordingly, temperature signals can be recorded from events back as far as the end of the last (Weichselian) glaciation. However, because of the diffusive character, the older the signal is the more it is attenuated with a corresponding larger uncertainty in magnitude and timing. By analysing the variation of temperature with depth (see section 1.2.2), one can reconstruct the past fluctuation at the Earth’s surface to a certain extent. The necessary technique is described in section 1.2.2.
1.1.4 Latent heat effects

When modelling heat transport in northern latitudes or in periods with freezing, it is necessary to consider latent heat effects due to freezing and thawing of pore water. This strongly affects the thermal regime, consuming or liberating large amounts of latent heat. This changes enthalpy by orders of magnitude, which requires a modification of the heat transport equation (1.17). This is discussed in chapter 3 since it plays a significant role when inverting borehole data for ground surface temperature histories.

1.2 Forward and inverse modelling techniques

 Generally, modelling physical processes requires first a discretisation of the domain to be studied ("gridding"), assigning available scalar and vector properties to the grid nodes. This is achieved by different discretisation schemes, such as finite elements, finite volumes, or finite differences which are used here. Then the governing differential equations need to be solved on the grid or mesh which is accomplished by appropriate algorithms. For the inverse problem, being ill-posed in general, forward modelling is necessary as well, but finding the best models in terms of data fit requires additional different sophisticated techniques.

1.2.1 Forward modelling

In this dissertation, SHEMAT (Simulator for HEat and MAss Transport, [Clauser (2003)]) is used for numerical forward simulation of heat and mass flow. It is a general-purpose, reactive transport simulation code for a wide variety of thermal and hydrogeological problems in two and three dimensions. Specifically, SHEMAT solves coupled problems involving fluid flow, heat transfer, species transport, and chemical water-rock interaction in fluid-saturated porous media. It can handle a wide range of time scales. Therefore, it is useful to address both technical and geological processes. Here, it is used to solve equa-
tion (1.17a) for transient problems, and equation (1.17b) for steady-state problems. The work in hand extends the application field to thermal systems where freezing processes become important (see chapter 3). SHEMAT uses a finite difference (FD) method to solve the partial differential equations. Three schemes are available for the spatial discretisation of the advection term in the transport equations: a pure upwind scheme, the Il’in flux blending scheme (Il’in, 1969) and the Smolarkiewicz diffusion corrected upwind scheme (Smolarkiewicz, 1983). The resulting system of equations can be solved explicitly, implicitly or semi-implicitly. For implicit and semi-implicit time-weighting the sets of linear equations can be solved by a variety of direct or iterative methods.

1.2.2 Inverse modelling

As outlined in section 1.1.3 ground surface temperatures (GST) are directly related to past temperatures. This makes them potentially valuable in analysing past climatic conditions. Most algorithms commonly used for ground surface temperature history inversion assume a one-dimensional, purely conductive model. The physical properties are known and the medium is either layered (Shen and Beck, 1991, 1992) or homogenous (Beltrami and Mareschal, 1995). Both algorithms use analytical functions to calculate transient disturbances to the subsurface. However, in this work a new, versatile 1-D inversion technique based on a FD approach is used. It allows to fully implement any nonlinear dependencies of thermal properties, such as the latent heat effect (see chapter 3).

There is no unique solution for the inverse problem of finding a GST history from geothermal measurements. Noise in the data adds further complications. Two different inverse approaches are applied here, using the same FD method for solving the forward problem: (1) a systematic inversion, meaning that an objective function is defined which has to be minimised using a Tikhonov regularisation of variable order for the generally ill-posed problem; (2) The Monte Carlo method which explores the model space fully by randomly varying the parameters subject to certain conditions.

Tikhonov inversion

Given recent borehole temperatures as a function of depth, $T(z)$, the GST history $T(0,t)$ can be estimated by a regularised least-squares procedure. To this end, an objective function $\Theta$ is set up to be minimised:

$$\Omega = ||W_d (d - g(p))||_2^2 + \sum_{i=0}^{M} \tau_i ||W_p (p - p_a)||_2^2$$  \hspace{1cm} (1.18)

Here $d - g(p) \equiv r$ is the residual vector between the data $d$ and the solution of the forward problem $g(p)$ for a given parameter vector $p$. The weighted (Euclidian) 2-norm of this residual represents the data fit. Data weighting is introduced by $W_d$ which is usually used to standardise the residuals, i.e. it is set to the inverse square root of the data covariance. The second term in equation (1.18) is defined by the application of $M$ linear operators $W$ on the deviations of the model parameters $p$ from their preferred values $p_a$. Regularisation is necessary in solving inverse problems because the simple least-squares solution (first term in equation 1.18) is completely dominated by contributions from data errors and rounding errors. $\tau$ is trade-off parameter to be determined, which improves the conditioning of the problem, thus enabling a numerical solution. In some cases $W_p$ can often be related to the square root of the inverse of some parameter a priori covariance.
To solve the inverse problem, the minimum of functional (1.18) is sought. If \( p^n \) is the current model at time \( n \), then a linear Taylor series approximation of the data for the model to be found at this iteration is

\[
g^{n+1} \approx g^n + J^n \delta p^n
\]  

(1.19)

where \( g^n = g(p^n) \), \( \delta p = \delta p^{n+1} - \delta p^n \), and \( J \) is the Jacobian matrix of sensitivities. It is defined as:

\[
J_{ij} = \frac{\partial g_i}{\partial p_j}.
\]

Using equation (1.19) in the objective function (1.18) changes to:

\[
\Omega(p^{n+1}) \approx \|W_d(d - g(p^n) - J^n \delta p)\|^2_2 + \sum_{i=0}^M \tau_i \|W_p^i(p - p_a)\|^2_2.
\]  

(1.20)

This expression is differentiated with respect to the elements of \( \delta p \). Equating the resulting equations (whose number is the number of model parameters) to zero yields the following linear system of equations to solve:

\[
\left( (W_dJ)^T W_dJ + \sum_{i=0}^M \tau_i (W_p^i)^T W_p^i \right) \delta p = W_dJ^T r - \sum_{i=0}^M \tau_i (W_p^i)^T W_p^i (p + p_a).
\]  

(1.21)

Differentiation is done by a perturbation method, using a very general FD solver, as mentioned above. Joint inversion of multiple data sets is easily achieved either by using appropriate priors (e.g., a well-understood borehole in the region) for every single borehole or by direct concatenation of Jacobians as shown in figure (1.2) below.

\[\text{Fig. 1.2: Schematic figure explaining the setup of the Jacobian in joint inversion.}\]
To solve the linear system equation (1.21), an equivalent formulation can be found which is very flexible and allows using a variant of the well-known conjugate gradient method for its solution:

\[
\begin{bmatrix}
W_d J \\
\tau_0 W_0^p \\
\tau_1 W_1^p \\
\vdots \\
\delta p
\end{bmatrix} =
\begin{bmatrix}
W_d^T (d - g(p)) \\
-\tau_0 W_0^p (p - p_a) \\
-\tau_1 W_1^p (p - p_a) \\
\vdots
\end{bmatrix}.
\] (1.22)

This rectangular system of linear equations is efficiently solved in each iteration by conjugate gradient least squares methods (CGLS) (e.g., Hansen, 1999; Aster et al., 2004). For ill-posed problems it is well known that this method regularises when truncated after a few iterations. On the other hand, it shows a semi-convergent behaviour at later iterations. In this implementation, the CGLS algorithm is complemented by a new stopping rule given by Berglund (2002).

In the case of GSTH inversion, the surface temperatures are parameterised as a series of step functions for \( p \). Number and temporal spacing of steps are set a priori, leaving the temperature values for each period as inversion parameters. These parameters are associated to the time steps indirectly. The time discretisation of the forward problem thus can be chosen following numerical requirements, independently from the inverse grid employed. Due to the diffusive character of the underlying physics, the use of a graded mesh in time and space is useful to reduce computing times.

For an equidistant temporal discretisation, these may be defined as

\[
W_0^p = I \quad W_1^p = (\Delta t)^{-1} \begin{bmatrix}
-1 & 1 & \cdots & 0 \\
-1 & 1 \\
\vdots \\
0 & -1 & 1
\end{bmatrix} \quad W_2^p = (\Delta t^{-2}) \begin{bmatrix}
1 & -2 & 1 & \cdots & 0 \\
1 & -2 & 1 \\
\vdots \\
0 & 1 & -2 & 1
\end{bmatrix}.
\] (1.23)

The product of these matrices with the parameter vector \( p \) may be interpreted as discrete approximations of the first and second derivative, respectively. \( \Delta t \) is the discretisation in time. It is straightforward to construct a Laplacian operator in the same manner but this study uses exclusively the \( W_1^p \) and the diagonal regularisers. There is a close connection of these difference operators to the covariances used in Bayesian theory. It has been pointed out (Tarantola, 1987; Yanovskaya and Ditmar, 1990; Xu, 2005; Tarantola, 2004), that the inverse of the exponential covariance may be represented approximately by a weighted sum of a diagonal and the squared \( W_1^p \) matrix. For a given data set and parameterisation, the optimal regularisation parameters \( \tau_i \) may be found by experiment, by using an L-curve approach (Hansen, 1999; Hartmann et al., 2005), or by the generalised cross validation (GCV) criterion (Wahba, 1990; Hansen, 1999). The detailed illustration of this method is given in chapter 4.

**Monte Carlo inversion**

The Monte Carlo method tests randomly selected combinations of surface temperature histories, heat flow, and present ground surface temperatures by using them as input for a forward model. It is a highly dimensional space of models: The GST history is divided in \( N \) step changes of surface temperature \( \Delta T \); together with specific heat flow and present GST the model space is \( N+2 \) dimensional. In contrast to other
works using Monte Carlo methods for determining GST histories (e.g. \cite{Kukkonen_Joeleht_2003, Dahl-Jensen_1998}, the forward problem is not solved by an analytic expression, but by finite differences which considerably increases computing times. On the other hand, this allows to implement fully any (nonlinear) features of the associated thermophysical properties as described above. Thus, the number of step changes \( N \) must be kept small, as well as the number of calculated forward models. For geothermal lithospheric studies, \cite{Jokinen_Kukkonen_1999} and \cite{Jokinen_Kukkonen_2000} use 1-D and 2-D finite difference codes for Monte Carlo inversions.

In an inversion run, as a first step a random GST history is sampled. From this, the corresponding temperature gradient is calculated, which subsequently is tested against the data (\cite{Mosegaard_Tarantola_1995}):

\[
S(p) = \frac{1}{2} \sum_{i=1}^{N} \left( \frac{\partial g^i}{\partial z}(m) - \frac{\partial d^i}{\partial z} \right)^2.
\]  

(1.24)

Starting from the given model a new random one is generated iteratively, with the parameters constrained appropriately. In this case, box constraints of \( \pm 2 \text{ K} \) are used with respect to the old model. For this model, the misfit \( S \) is calculated according to (1.24). If the new misfit \( S_{\text{new}} \) is smaller than the misfit \( S_{\text{old}} \) of the previous model, the change is accepted. However, even if the new misfit is larger, the new model is accepted with a certain probability, so that the acceptance probability is:

\[
P_{\text{acc}} = \begin{cases} 
1 & \text{if } S(p_{\text{new}}) \leq S(p_{\text{old}}) \\
\exp\left(-\frac{S(p_{\text{new}})-S(p_{\text{old}})}{s^2}\right) & \text{if } S(p_{\text{new}}) > S(p_{\text{old}})
\end{cases},
\]

(1.25)

where \( s^2 \) is the noise variance of the data, in the case of Gaussian uncertainties. This is the so called Metropolis algorithm (\cite{Mosegaard_Tarantola_1995}) which ensures that the model space is fully sampled, and avoids getting stuck in local minima.

1.3 State of the art

Specific heat flow profiles derived from thermophysical measurements in boreholes in moderate to high latitudes very often feature a vertical variation, such as those from the Kola super-deep borehole, other deep boreholes in Russia, and from the KTB boreholes (\cite{Popov_1998, Popov_1999b, Clauser_1997}). The vertical variation of specific heat flow with depth cannot be explained by purely steady-state heat conduction in the crust. Steady-state conduction of heat would imply a specific heat flow profile which decreases with depth according to the heat generation of rocks. Three main processes may have a potential major influence on the thermal regime in the upper crust: (1) Heterogeneity, i.e. variation of thermal and hydraulic rock properties with depth; (2) heat advection by fluid flow; (3) transient disturbances resulting from transient variations of the Earth’s ground surface temperature in the past. The vertical variation can also be induced by other processes like sedimentation, uplift, erosion, magmatic activity, or topography. In this work however, the focus lies on the former three processes. In order to study and quantify these effects, it is necessary to perform numerical simulations of heat transport and fluid flow, both in forward and inverse mode.

Concerning the area around the Kola super-deep borehole, earlier results suggest in particular an important influence of advective and refractive effects in addition to palaeoclimate (\cite{Kukkonen_Clauser_1994}).
1.4 Outline and aim of this dissertation

This work contributes to the current efforts to quantify different processes potentially responsible for a vertical variation of specific heat flow. To this end, numerical forward and inverse modelling is applied.

A large data set from the Kola peninsula forms the basis for studying the influence of heterogeneity, fluid flow, and palaeoclimatic by numerical simulations. The results of this case study allow to quantify of these processes to a certain extent. After a general introduction in chapter 1, the presentation and discussion of the data, as well as the results of numerical 3-D simulations is the topic of chapter 2. While the numerical modelling in chapter 2 is performed in the forward mode, chapter 3 presents results from inverse simulations, addressing the reconstruction of past temperatures back to the last ice age.
In contrast to most inverse algorithms (see previous section), the method applied here is based on finite differences and can include any (nonlinear) physics. Therefore, it was possible to include the effects of developing and decaying permafrost in both forward and inverse simulations. This has been carried out within the framework of this dissertation since it is essential to account for permafrost effects when studying middle and high latitude borehole temperatures. In the course of this study the associated effects turned out be potentially significant for subsurface temperatures. In particular, porosity is a critical parameter. Since these effects are negligible in the crystalline environment of the Kola area, borehole data from the northern Poland is used to demonstrate the impact of the latent heat effects associated with permafrost on palaeotemperature reconstructions.

Information on past climate changes is crucial when predicting the future of the Earth’s surface temperature. The inclusion of latent heat effects in palaeotemperature inversions is a new approach which helps to characterise past temperatures in areas with present or past subsurface freezing conditions. Since this may possibly modify results from earlier GST history inversions, it motivated another study which aims at a general characterisation of the influence of latent heat effects on GST history inversions. This required a large number of inverse simulations with different models and parameters, therefore an automatic determination of the regularisation parameters turned out to be inevitable. The applied method based on the the generalised cross validation criterion is a novel approach for palaeoclimatic inversions. Its implementation in the inverse code and its application to synthetic and field data is thus described in a separate chapter. The general study, which enables to assess the deviation of earlier inversion results neglecting latent heat effects, is presented in chapter.

Chapter summarises the main issues of this work and presents an outline for future work.
2. HEAT TRANSPORT PROCESSES IN THE UPPER CRUST NEAR THE KOLA SUPER-DEEP BOREHOLE

This chapter presents a case study of heat transfer processes in the Earth’s upper crust. From a field campaign to the immediate vicinity of the Kola super-deep borehole on the Kola peninsula and subsequent petrophysical measurements, a large data set could be obtained which is used in this dissertation. It comprises temperature logs and petrophysical measurements on samples from 36 boreholes of up to 1.6 km depth. This data set is presented in the first part of this chapter and forms the basis for a 3-D model which allows to quantify the different influences on crustal heat flow described in the second part of the chapter. Parts of this chapter are published in Mottaghy et al. (2005).

2.1 Geological setting of the Kola super-deep borehole

The Kola super-deep borehole SG-3 is located on the northern rim of the Fennoscandian (Baltic) Shield at 69°23’N, 30°36’E. It is the deepest borehole in the world to date. Situated in the Pechenga ore district, its distance to the Barents Sea is about 50 km (figure 2.1). The landscape modified by Weichselian and earlier glaciations has a mean elevation of about 1.5 m – 300 m above sea level. Its bedrock of Proterozoic and Archaean age is covered by Quaternary glacial deposits, typically only a few metres thick at most. The Proterozoic rocks consist mainly of mafic and ultramafic metavolcanic and igneous rocks, and metasediments in a synclinal structure within the Archaean gneiss complex. Archaean rocks are mostly acidic and intermediate gneisses and amphibolites.

2.2 Data

There is data available from altogether 36 boreholes, 34 of which are in the vicinity of the super-deep borehole, one is located 10 km to the north, and one 50 km to the south of SG-3 in the Allarechenskii district. Measurements of borehole temperatures were performed in the 1 km – 2 km deep holes and of rock thermal properties and hydraulic permeabilities on core samples. 22 temperature logs recorded between 1960–1980 were re-evaluated and digitised. The remaining 14 new logs were measured in 1994. The holes had been diamond drilled with diameters less than 70 mm. Most of the logs show an increase of inclination with depth. Where inclination data was available, the logs were corrected to true depth. This was possible for 10 of the 14 new logs and for 17 of the 22 old logs. Core was obtained from 23 boreholes, not only from the boreholes logged in 1994, but also from those holes logged from 1960–1980. Table 2.2 summarises the available data on all considered boreholes.
<table>
<thead>
<tr>
<th>No.</th>
<th>Borehole</th>
<th>Longitude (° east)</th>
<th>Latitude (° north)</th>
<th>Depth (m)</th>
<th>Elevation (m)</th>
<th>Gradient</th>
<th>To Thermal Conductivity</th>
<th>Specific heat flow (W/mK)</th>
<th>Specific heat (J/kgK)</th>
<th>Heat (W/m^2)</th>
<th>Range (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>32</td>
<td>2.9 ± 0.2</td>
<td>32</td>
<td>90.0 ± 1.6</td>
<td>69.9 ± 0.0</td>
<td>11</td>
<td>1.0 ± 10.1</td>
<td>99.0 ± 4.9</td>
<td>13</td>
<td>30.5</td>
<td>90.5</td>
</tr>
<tr>
<td>2</td>
<td>32</td>
<td>2.9 ± 0.2</td>
<td>32</td>
<td>90.0 ± 1.6</td>
<td>69.9 ± 0.0</td>
<td>11</td>
<td>1.0 ± 10.1</td>
<td>99.0 ± 4.9</td>
<td>13</td>
<td>30.5</td>
<td>90.5</td>
</tr>
<tr>
<td>3</td>
<td>32</td>
<td>2.9 ± 0.2</td>
<td>32</td>
<td>90.0 ± 1.6</td>
<td>69.9 ± 0.0</td>
<td>11</td>
<td>1.0 ± 10.1</td>
<td>99.0 ± 4.9</td>
<td>13</td>
<td>30.5</td>
<td>90.5</td>
</tr>
<tr>
<td>4</td>
<td>32</td>
<td>2.9 ± 0.2</td>
<td>32</td>
<td>90.0 ± 1.6</td>
<td>69.9 ± 0.0</td>
<td>11</td>
<td>1.0 ± 10.1</td>
<td>99.0 ± 4.9</td>
<td>13</td>
<td>30.5</td>
<td>90.5</td>
</tr>
<tr>
<td>5</td>
<td>32</td>
<td>2.9 ± 0.2</td>
<td>32</td>
<td>90.0 ± 1.6</td>
<td>69.9 ± 0.0</td>
<td>11</td>
<td>1.0 ± 10.1</td>
<td>99.0 ± 4.9</td>
<td>13</td>
<td>30.5</td>
<td>90.5</td>
</tr>
<tr>
<td>6</td>
<td>32</td>
<td>2.9 ± 0.2</td>
<td>32</td>
<td>90.0 ± 1.6</td>
<td>69.9 ± 0.0</td>
<td>11</td>
<td>1.0 ± 10.1</td>
<td>99.0 ± 4.9</td>
<td>13</td>
<td>30.5</td>
<td>90.5</td>
</tr>
</tbody>
</table>

**Table 2.1: Overview of data on the Kola shallow boreholes.**

*No data where logged in/prior to 1994

---

3. Heat transport processes in the upper crust near the Kola super-deep borehole
2.2. Data

2.2.1 Thermal conductivity

A very detailed study on thermal conductivity with respect to anisotropy, inhomogeneity and temperature dependence was performed, examining cores of 21 boreholes at a depth interval of 10 m.

Tensor components of thermal conductivity were determined on 1375 core samples from 21 boreholes in 3400 measurements at ambient temperature using the optical scanning method. A detailed description and comparison with other methods can be found in (Popov et al., 1999c). This method is both fast and reliable with an accuracy of ±3%. For all samples studied the precision was 2%.

The optical scanning lines were oriented parallel and perpendicular to foliation, bedding or stratification on sawed flat surfaces of the core samples. The length and the diameter of the cores varied from 6 cm – 15 cm and 4 cm – 7 cm, respectively. Measurements were performed on dry rocks since, according to theoretical findings (Popov and Mandel, 1998), the influence of water saturation can be neglected due to porosities below 1% (see section 2.2.4). The variation of thermal conductivity was recorded on two to five different scanning lines in each of two perpendicular directions. Lines of black paint (thickness: 25 µm – 40 µm) were applied on each scanning line in order to obtain comparable optical properties for all samples.

The average of the apparent thermal conductivity values resulting from several scanning lines $i$ were used to calculate the thermal conductivity parallel and perpendicular to stratification, bedding or foliation, $\lambda_{par}$ and $\lambda_{per}$, respectively. Thus, the coefficient of anisotropy $K = \lambda_{par}/\lambda_{per}$ can be calculated. Further, an inhomogeneity factor $\beta = (\lambda_{max} - \lambda_{min})/\lambda_{ave}$ can be defined, consisting of the maximum, minimum and average apparent thermal conductivity of each line, $\lambda_{min}$, $\lambda_{max}$, and $\lambda_{ave}$, respectively. This parameter $\beta$ characterises the inhomogeneity of a rock sample, which is useful for petrophysical and geothermal investigations (Popov and Mandel, 1998).

As an example, figure 2.2 shows the results obtained for borehole 1800, with respect to thermal conductivity tensor components, anisotropy coefficient $K$, and thermal inhomogeneity factor $\beta$.
1. Heat transport processes in the upper crust near the Kola super-deep borehole

Using the detailed information on the tensor components, Popov and Mandel (1998) developed an algorithm for calculating the conductive specific heat flow in anisotropic rock for various combinations of the orientations of the principal axes of the thermal conductivity tensor and of the temperature gradient (see section 2.2.2). An effective thermal conductivity $\lambda_{\text{eff}}$ takes into account that the terrestrial specific heat flow may deviate from the vertical:

$$\lambda_{\text{eff}} = \sqrt{\lambda_{\text{per}}^2 \cos^2 \varphi + \lambda_{\text{par}}^2 \sin^2 \varphi},$$

(2.1)

where $\varphi$ is the angle of stratification or foliation (dip angle). $\lambda_{\text{eff}}$ was calculated for each core by determining $\lambda_{\text{par}}$, $\lambda_{\text{per}}$ and dip angles $\varphi$. Accounting for the tensor character of thermal conductivity helps to avoid a systematic error of up to 13 %, which would appear at typical values of rocks in the Kola region with anisotropy coefficients of 1.5 and dip angles of 45°.

Thermal conductivity $\lambda$ was determined for all existing lithologies in the study area. Figure 2.3b summarises the results of all measurements in terms of thermal conductivity $\lambda$, anisotropy coefficient $K$, and thermal inhomogeneity factor $\beta$ for the rock types studied; Figure 2.3a contains also data from the SG-3 borehole. The lithologies in figure 2.3 were characterised by Russian researchers on samples from both the super–deep hole and the shallow holes. However, in the course of the more recent measurements, main lithologic units were determined from the samples of the shallow holes, using thin sections and x-ray fluorescence analysis. Therefore, this classification differs somewhat from the older one (see below and section 2.2.4). For most boreholes the effective thermal conductivity $\lambda_{\text{eff}}$ varies between 2 W m$^{-1}$ K$^{-1}$ – 5 W m$^{-1}$ K$^{-1}$ (figure 2.3a). There are considerable local variations in $\lambda_{\text{eff}}$ and $K$ as well as trends along the boreholes. Thus, obtaining a great number of measurements of the tensor components of the thermal conductivity is crucial in order to obtain reliable data for calculating specific heat flow and its vertical variation.
2.2. Data

The principal components $\lambda_{\text{par}}$ and $\lambda_{\text{per}}$ of the thermal conductivity tensor all fall within the range $1.7 \text{ W m}^{-1} \text{K}^{-1} - 6.3 \text{ W m}^{-1} \text{K}^{-1}$. 40% of the studied cores show a significant degree of anisotropy ($1.0 \leq K \leq 2.0$). Figure 2.3 illustrates that in most cases the thermal conductivity tensor component parallel to the macroscopic foliation (or bedding) $\lambda_{\text{par}}$ was larger than the perpendicular component $\lambda_{\text{per}}$. In those cases which show opposite behaviour, thin sections of 12 samples from different depth intervals were studied additionally. The result is shown in figure 2.4. Sheets of mica and chlorite of great anisotropy are oriented at an oblique or normal angle to the foliation and bedding plane. This can be attributed to a younger foliation developed after the main (macroscopically observable) bedding or foliation. With this additional information the real directions of the principal axes of thermal conductivity could be determined. No cores were available from the ore-bearing sections. Thermal conductivity of ore could only be studied on a small collection of rock samples in a preliminary way. In order to obtain more reliable data, measurements on ore samples from other ore deposits were performed, which were similar in genesis and mineralogic composition to the strata dealt with in this study (Romushkevich and Popov, 1998). Thermal conductivity values of these samples vary from $3.7 \text{ m}^{-1} \text{K}^{-1} - 9.8 \text{ W m}^{-1} \text{K}^{-1}$. The massive and mottled ores of pyrrhotite-pentlandite-chalcopyrite composition are characterised by a high thermal conductivity. Relatively low values are typical for disseminated ore. Thermal conductivity of mineralised phyllite (little veins and disseminations) is $3.2 \text{ W m}^{-1} \text{K}^{-1}$.

Temperature dependence of thermal conductivity

The variation of thermal conductivity with temperature was determined on a small subset of rock samples up to 100 °C (some up to 300 °C) using the divided bar method. This temperature range was chosen with
2. Heat transport processes in the upper crust near the Kola super-deep borehole

Fig. 2.4: Microscopic image (Popov et al., 1999a) of thin section of chlorite with a high degree of thermal anisotropy: the component parallel to the bedding structure is smaller than the perpendicular component.

respect to future modelling, allowing to determine thermal conductivity down to about 8 km – 9 km (see section 2.2.2). Thermal conductivity varies inversely with temperature up to several 100 °C, as described in section 1.1.1. Results were fitted to equation 1.12 by determining the coefficients a and b for samples of nine boreholes including different lithologic units (table 2.2). The general uncertainty of divided bar measurements is ±3 %, which is marked by error bars on the data points in figure 2.5. It shows an example for a serpentinite sample with intercalated tuff layers. Figure 2.5 also shows λ(T) for the seven main lithologic units. Following Lubimova et al. (1985) and Popov et al. (1999b), it was concluded that the total correction for temperature can be neglected for depths of up to 2000 m and thus for this study. However, if any corrections were applied, they would be in the temperature range below 20 °C as the average annual surface temperature at the SG-3 site is 0.5 °C – 1 °C and the average temperature gradient is about 11 K km⁻¹ (see section 2.2.2). The laboratory measurements were carried out at about 20 °C, and thus the resulting correction would be positive. However, applying equation 1.12 to a sample from borehole 3200, the change in thermal conductivity due to temperature differences in that range turned out to be smaller than ±3 %, the accuracy of the optical scanning and divided bar apparatuses.

2.2.2 Temperature gradient

In the period from 1960–1980 Soviet researchers recorded a considerable number of temperature logs. As these records are available as paper plots only, their reliability and degree of disturbance can only be estimated by visual inspection. These single-point measurements at a 5 m – 10 m interval turned out to be of generally good quality. Those 22 of the available logs in the Pechenga area were selected, which seemed to be least disturbed. These paper logs were digitised. Some logs had been originally corrected for inclination, however only at very long depth intervals. The correction at an interval of 5 m could be applied in greater detail with the available data. The maximum depth deviation between the "old" and
### Tab. 2.2: Coefficients for determining the variation of thermal conductivity with temperature as in equation 1.12

<table>
<thead>
<tr>
<th>Borehole</th>
<th>Depth m</th>
<th>a × 10^4 (W m⁻¹)</th>
<th>b × 10^1 (W K m⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1553</td>
<td>317</td>
<td>0.718463</td>
<td>3.863014</td>
</tr>
<tr>
<td>3200</td>
<td>612</td>
<td>1.029461</td>
<td>3.001504</td>
</tr>
<tr>
<td>3200</td>
<td>905</td>
<td>0.8791</td>
<td>2.709893</td>
</tr>
<tr>
<td>3200</td>
<td>1164</td>
<td>2.030282</td>
<td>2.470183</td>
</tr>
<tr>
<td>3200</td>
<td>1222</td>
<td>1.354836</td>
<td>3.27906</td>
</tr>
<tr>
<td>3200</td>
<td>1325</td>
<td>1.131005</td>
<td>2.956288</td>
</tr>
<tr>
<td>3396</td>
<td>320</td>
<td>1.580787</td>
<td>3.022084</td>
</tr>
<tr>
<td>3396</td>
<td>600</td>
<td>1.46958</td>
<td>3.647177</td>
</tr>
<tr>
<td>3396</td>
<td>1240</td>
<td>1.293651</td>
<td>3.560495</td>
</tr>
</tbody>
</table>

**Fig. 2.5:** Left: Variation of thermal conductivity with temperature T for a sample of serpentinite with tuff intercalations from a depth of 1164 m in borehole 3200. Error bars indicate the uncertainty of the measurement of ±3%. Right: Variation of thermal conductivity with temperature T for all existing lithologies in the study area. Error bars and data points are omitted in favour of better viewing.
In 1994, new temperature logs were recorded in 14 boreholes in the Kola region (figure 2.6). The holes were all in thermal equilibrium as they had been at rest for several years. Measurements were continuous logs and point measurements with Analog Device AD 590 chip probes at a resolution of ±10 mK and an accuracy of ±100 mK. Ten of these logs could be corrected for inclination.

“new” corrections amounted to as much as 40 m in a few cases. The total maximum depth correction for a 1400 m borehole is more than 100 m. For four boreholes there is no inclination data.

Fig. 2.6: 14 temperature logs recorded in the summer of 1994. Logs are offset by 3 K for easier viewing.

Fig. 2.7: Reduced temperature profiles calculated for the 14 temperature logs of figure 2.6 for a constant surface temperature of 1 K and a vertical temperature gradient of 11 K km$^{-1}$. Logs are offset by 1 K.
The vertical component of the temperature gradient $\partial T / \partial z$ was first determined from finite differences, and then smoothed by a moving average. This removes the high-frequency scatter introduced by the finite differences which is caused by the high resolutions in depth and temperature of 0.03 m and 10 mK, respectively. When measuring temperature at points one meter apart at a temperature gradient of about 10 K km$^{-1}$, the resolution of the borehole thermometer is reached. Therefore, the temperature gradient was calculated at 5 m interval by applying a distance-weighted moving average over an interval of ± 50 m. The mean temperature gradient of the study area is about 11 K km$^{-1}$. This rather low regional average of the temperature gradient is due to great age (over 2000 Ma) of the bedrock in the area.

In order to determine mean specific heat flows for each borehole, a constant temperature gradient was calculated over an interval by linear regression of the temperature log. Each depth range was selected with respect to the quality of the temperature log and negligible influences from surface, structural, or advective effects. To this end, reduced temperature logs were calculated assuming a constant surface temperature of 1 K and a vertical temperature gradient of 11 K km$^{-1}$. Figure 2.7 shows the reduced temperature logs recorded in 1994, offset from each other by 1 K for better viewing. Table 2.2 lists the results for all boreholes.

2.2.3 Specific heat flow

The vertical variations of specific heat flow were determined – except for borehole 1789 – by combining temperature gradient and thermal conductivity for depth intervals of 5 m in each well. Thermal conductivity is usually not available at an equidistant interval. A moving harmonic average is used for equidistant data interpolation. Because there is no thermal conductivity for borehole 1789, mean thermal conductivity values were used according to the major lithologies. As described in section 2.2.1 an effective thermal conductivity is used to calculate the modulus of heat flow in an anisotropic rock according to equation 1.3, which becomes here

$$q_i = -\lambda_{eff,i} \frac{\Delta T_i}{\Delta z_i}.$$  (2.2)

The subscript $i$ indicates a particular depth according to the equidistant increment $\Delta z$. As an example figure 2.8 shows a composite log of borehole 3356. The vertical white bar in the specific heat flow graph indicates the depth range over which a single value of specific heat flow was determined. As described in 2.2.2 for each borehole a different depth interval was chosen, where the temperature log was least disturbed. Additionally, the vertical variation of specific heat flow is also used for defining this depth interval, because sharp changes in thermal conductivity must be avoided. Three methods were applied to calculate specific heat flow, the "Bullard method" and two "interval methods", using different ways to determine the temperature gradients (results and data: see table 2.2):

1. Assuming steady state and conductive specific heat flow with negligible heat sources and sinks, the variation of temperature $T(z)$ with depth can be expressed by (Bullard, 1939)

$$T(z) = T_0 - q_0 \sum_{i=0}^{n} (\Delta z_i / \lambda_i).$$  (2.3)

The ratio $\Delta z_i / \lambda_i$ is often called thermal resistance. The partial derivative in equation (1.1) is re-
2. The vertical variations of the temperature gradient and the thermal conductivity obtained for each hole (left and centre panel in figure 2.8, solid lines) were averaged arithmetically over the same depth range and multiplied. Here the error is the root-mean-square.

3. The interval method uses the temperature gradient values determined by linear regression over the depth range in question:

\[ T(z) = T_0 + mT \]  

(2.4)

The parameter \( m \), the slope or gradient, is shown in table 2.2 the associated error results from the standard deviation of the slope in the least square fit. Since values for the ground surface temperature obtained by the Bullard method do not differ much from this method, \( T_0 \) from equation (2.4) is shown in table 2.2 for each borehole. The mean thermal conductivity is the harmonic mean of the individual values within the regarded depth range. The error in specific heat flow is determined by propagation of the errors in thermal conductivity and temperature gradient.

The difference between the three different methods amounts to 2 mW m\(^{-2}\) at maximum, well within the error range of specific heat flow (see table 2.2). All specific heat flow values fall within the range of 31 mW m\(^{-2}\) to 45 mW m\(^{-2}\) with an average of 38 mW m\(^{-2}\).
2.2. Data

Figure 2.9 shows the distribution of boreholes in the study area. Specific heat flow values are indicated at those where all necessary data is available. Other boreholes are marked by triangles.

2.2.4 Other petrophysical data

Other petrophysical properties were determined on various subsets of 55 core samples from 16 boreholes. These samples represent the seven main lithologic units of the study area which were determined as described above: gneiss, ultramafites/ultrabasites (pyroxenite), sediments (clay- and sandstones), basic magmatic rocks (gabbro diabase), volcanic rocks (tuff, tuffites), picrite and amphibolites.

Density

Water saturated bulk density \( \rho_b \) (including pore space) and rock density \( \rho_0 \) (without pore space) were measured on 25 samples (figure 2.10), representing all seven main rock types. Sample mass was measured with laboratory scales and sample volume with a helium pycnometer for determining rock density. The uncertainty of this method is \( \pm 0.06 \% \). In order to obtain bulk density, a displacement technique was applied, which uses a fine powder to determine total volume. This method has an uncertainty of \( \pm 1.1 \% \).

Porosity

Porosity \( \Phi \) was determined from both bulk and rock density according to

\[
\phi = 1 - \frac{\rho_0}{\rho_b}.
\]  

(2.5)
2. Heat transport processes in the upper crust near the Kola super-deep borehole

In view of the small differences between both densities, it is evident that porosity is very small. Figure 2.10 shows the results.

Permeability

The variation of permeability as a function of pressure was measured using a transient gradient method in an autoclave. Roughly 50 rock samples were studied, which again represent the main rock types. The confining pressure can reach 300 MPa, but to simulate in situ situations of the Kola core samples 80 MPa are sufficient. For borehole 3396 the permeability for the lithologic gneiss unit was measured in terms of depth and thus pressure. Only this rock type and gabbro yielded a significant variation of permeability with pressure. All other samples have very low permeability, with values near the detection limit of $10^{-21}$ m$^2$ of the apparatus.

The near-surface gneiss samples of borehole 3396 show less pressure dependence than those from greater depth. This depends on lithology and texture, because the shallow gneiss is coloured by dark mica and foliated, while the deeper gneiss is light, isotropic, and inhomogeneous in grain size distribution. Additionally, this gneiss shows visible fissures which had been coloured red by circulating waters. Hence, both types of gneiss behave differently in terms of crack closure due to pressure. The variation of permeability $k$ with pressure $p$ can be represented by two different exponential functions (figure 2.11): $ln(k) = -0.5ln(p) + 3$ for the samples with little variation with pressure (40 m and 590 m depth) and $ln(k) = -1.7ln(p) + 6$ for those with a significant pressure dependence (680 m, 780 m, 1210 m).
\[ \ln(k) = -0.5 \ln(p) + a \]
\[ \ln(k) = -1.7 \ln(p) + b \]

**Fig. 2.11:** Variation of permeability with pressure and depth for samples from borehole 3396. The logarithmic functions describe the permeability of rock samples from different depths.

**Specific heat capacity**

With regard to future modelling it was necessary to determine the temperature dependence of isobaric specific heat capacity $c_P$ on 26 rock samples from 7 boreholes over a temperature range of $1^\circ C - 100^\circ C$. For these measurements a dynamic heat flow difference calorimeter was used. Data was recorded every 100 mK at a heating rate of 200 mK/min. The uncertainty of this method is $\pm 1\%$. The specific heat capacity is fitted to equation 1.13. The coefficients $A_0$, $A_1$, and $A_2$ are listed in table 2.3 for all samples. Figure 2.12 shows the results at ambient temperature for all rock types (left) as well as the number of the samples (right). Figure 2.13 illustrates the variation with temperature of thermal capacity, the product of density and specific heat capacity. Continuous lines are drawn and error bars are omitted, since the number of data points is very large.

**Thermal diffusivity**

Transient heat transport is governed by thermal diffusivity. Therefore it is of particular importance for the propagation of temperature variations such as those at the Earth’s surface due to palaeoclimatic changes. It is a function of thermal conductivity, density, and specific heat capacity (see also section 1.1.1):

\[ \kappa = \frac{\lambda}{\rho c_P} \] (2.6)

Its temperature dependence is rather significant. The reason is the opposite behaviour of thermal conductivity and heat capacity with respect to temperature. Between $1^\circ C - 10^\circ C$ thermal conductivity decreases by $4\% - 7\%$, while thermal diffusivity decreases by $18\% - 22\%$. Figure 2.14 shows the variation of thermal diffusivity with thermal conductivity at ambient temperature, the latter measured by the optical
### Borehole Depth Coefficients

<table>
<thead>
<tr>
<th>Borehole Depth (m)</th>
<th>Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$A_0 \times 10^{-2}$ (J kg$^{-1}$ K$^{-1}$)</td>
</tr>
<tr>
<td>1553 317</td>
<td>7.520180</td>
</tr>
<tr>
<td>1553 320</td>
<td>7.120666</td>
</tr>
<tr>
<td>1800 275</td>
<td>7.590378</td>
</tr>
<tr>
<td>1800 365</td>
<td>7.452511</td>
</tr>
<tr>
<td>1800 700</td>
<td>7.375681</td>
</tr>
<tr>
<td>1800 1400</td>
<td>7.245889</td>
</tr>
<tr>
<td>2330 690.5</td>
<td>8.830750</td>
</tr>
<tr>
<td>2400 525</td>
<td>8.291508</td>
</tr>
<tr>
<td>2908 890</td>
<td>8.386283</td>
</tr>
<tr>
<td>3200 50</td>
<td>7.498450</td>
</tr>
<tr>
<td>3200 275</td>
<td>7.323982</td>
</tr>
<tr>
<td>3200 612</td>
<td>7.481398</td>
</tr>
<tr>
<td>3200 905</td>
<td>7.428959</td>
</tr>
<tr>
<td>3200 1164</td>
<td>7.909242</td>
</tr>
<tr>
<td>3200 1222</td>
<td>7.115795</td>
</tr>
<tr>
<td>3200 1325</td>
<td>7.399932</td>
</tr>
<tr>
<td>3200 1338</td>
<td>7.305665</td>
</tr>
<tr>
<td>3200 1610</td>
<td>7.359384</td>
</tr>
<tr>
<td>3200 1692</td>
<td>7.285593</td>
</tr>
<tr>
<td>3396 40</td>
<td>7.228351</td>
</tr>
<tr>
<td>3396 310</td>
<td>7.163750</td>
</tr>
<tr>
<td>3396 320</td>
<td>7.143602</td>
</tr>
<tr>
<td>3396 590</td>
<td>7.309378</td>
</tr>
<tr>
<td>3396 600</td>
<td>7.130334</td>
</tr>
<tr>
<td>3396 1210</td>
<td>7.212732</td>
</tr>
<tr>
<td>3396 1240</td>
<td>7.155693</td>
</tr>
</tbody>
</table>

**Tab. 2.3:** Coefficients for determining the variation of the specific heat capacity with temperature as in equation 1.13.

![Diagram](image1)

**Fig. 2.12:** From left to right: Specific heat capacity, heat generation rate (the vertical dashed line specifies the threshold of the measurement method) and number of samples for the main rock types. In the case of amphibolite, the number of samples for $c_P$ (circle) and heat generation rate measurements (cross) are different.
scanning method. Data points are fitted by linear regression, including the origin:

$$\kappa = \frac{\lambda}{\rho c_p} = 0.44 \times 10^{-6} \frac{\lambda}{2.3 \times 10^6}. \quad (2.7)$$

Because of the self-compensating factors, the volumetric heat capacity $\rho c_p$ varies within 20 % of $2.3 \times 10^6$ J m$^{-3}$ K$^{-1}$ for the great majority of minerals and impervious rocks (Beck, 1988). In figure 2.15 the $\kappa$-$\lambda$ distribution is plotted at different temperatures ($\lambda$ from the divided bar measurements) up to 100 °C. The inverse of the slope of each of these linear regressions, $\rho c_p$, yields another linear relationship (figure 2.15), which allows to determine thermal diffusivity at any temperature, only based on the known temperature dependence of thermal conductivity:

$$\kappa(T) = f(\lambda(T)) = \lambda(T)/(0.0044 \ T + 2.134). \quad (2.8)$$

A similar relationship was developed by Vosteen and Schellschmidt (2003) for rock samples from eastern Alpine crystalline rocks.

**Heat generation rate**

The abundances of uranium, thorium, and potassium were determined by X-ray fluorescence analysis. Again, the samples were selected with respect to the main units. Figure 2.12 (centre) shows the results. The vertical dashed line marks the threshold of this method, which is 1.12 $\mu$W m$^{-3}$. When modelling the
Fig. 2.14: Thermal diffusivity versus thermal conductivity at ambient temperature.

Fig. 2.15: Left: Thermal diffusivity versus thermal conductivity at different temperatures. Right: Temperature dependence of the reciprocal slope $\rho c_p$. 
2.2. Data

Fig. 2.16: The vertical variation of specific heat flow vs. depth for all shallow holes (numbers) and for the super-deep borehole (SG-3) to a depth of 2 km. Almost all boreholes show an increase with depth, shown by a linear regression (grey line). One exception is borehole 3396 (topmost profile), which lies ≈50 km south of the Pechenga structure (discussion see text). Each profile is shifted by 20 mW m$^{-2}$.

thermal behaviour of the crust, this rather high limit leaves appreciable uncertainty. Thus, with respect to the numerical simulations, it was resorted to other data as well.

2.2.5 The vertical variation of specific heat flow

Earlier heat flow measurements in 10 boreholes in the surrounding of the super-deep Kola borehole yielded specific heat flow values from 28 mW m$^{-2}$ – 41 mW m$^{-2}$ with an average of 36 mW m$^{-2}$ (Arshavskaya et al. 1987). This study confirms these findings. However, no vertical variation of specific heat flow was reported at then.

Almost all boreholes show a significant increase of specific heat flow with depth. Although no borehole is deeper than 2 km, there is a significant trend below the depth of 10 m – 20 m where annual temperature oscillations vanish. Figure 2.16 shows specific heat flow logs of all boreholes, as well as data from the super-deep borehole SG-3, adapted from Popov et al. (1999b). Table 2.4 gives the coefficients $A$ and $B$ for those linear regressions $q(z) = A + Bz$ which are drawn in figure 2.16. The mean increase (heat flow gradient, $B = \partial q(z)/\partial z$) with depth is $13 \pm 8$ mW m$^{-2}$ km$^{-1}$. Specific heat flow values from table 2.2 were determined over a certain depth range which explains the deviation between these and $A$ in table 2.4. All values in table 2.2 lie within the range given by $q(z)$. 
2. Heat transport processes in the upper crust near the Kola super-deep borehole

2.3 Comparison with thermal data from the Kola super deep borehole

Additional information was obtained by comparison of the new data from shallow boreholes and data from the Kola super-deep borehole SG-3 (Popov et al., 1999b). A comparison of the thermal properties of rocks studied with those of cores from SG-3 (Popov et al., 1999a) shows that the thermal conductivity of rocks from the Pechenga ore field ranges from 1.3 W m\(^{-1}\) K\(^{-1}\) – 7.3 W m\(^{-1}\) K\(^{-1}\), which is almost the same range as in rocks from the SG-3 borehole (1.2 W m\(^{-1}\) K\(^{-1}\) – 7.3 W m\(^{-1}\) K\(^{-1}\)). From this it is concluded that complicated technological procedure of drilling the SG-3 borehole did not influence significantly core properties, with the exception of some depth intervals that will be discussed below. Diabase, intercalated sandstone, siltstone, and phyllite in both data sets have equal average thermal conductivity. The mean values for unaltered and actinolite diabases are also very similar for both data sets. The large thermal conductivity for the nickel-bearing intrusions in the Pechenga ore field compared to rocks from the SG-3 borehole are caused by their enrichment in sulfides. Table 2.5 and figure 2.3a indicate that the thermal conductivity of gneiss and amphibolite in the Archean complex from the shallow wells is larger by about 20 % compared to previous measurements on samples from the SG-3 borehole below 6800 m. This systematic difference is possibly due to the decompression and mechanical wear experienced by the cores from the SG-3 borehole. The temperature logs obtained in the Kola super-deep well SG-3 after 4 years of continuous shut-in time in 1998 (Popov et al., 1999b) were compared with temperature gradient values presented here. All temperature gradient data scatter around a general mean of 11±5 mK m\(^{-1}\). This is in good agreement with the variation of the temperature gradient from 11 mK m\(^{-1}\) to 16 mK m\(^{-1}\) observed in the top 2 km of the SG-3 borehole. The important conclusion is that the significant increase with depth in specific heat flow from 34 mW m\(^{-2}\) – 36 mW m\(^{-2}\) to 55 mW m\(^{-2}\) – 58 mW m\(^{-2}\) in the top 2 km of the SG-3 hole (see figure 2.16) are not caused by technical operations in the hole but reflect a natural process, most probably either lateral steady-state heat transfer due to anisotropy, inhomogeneity, and topography, fluid flow, palaeoclimate, or a combination of all.

<table>
<thead>
<tr>
<th>Borehole</th>
<th>A (mW m(^{-2}))</th>
<th>B (mW m(^{-3}))</th>
<th>Values from table 2.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>3396</td>
<td>38.5</td>
<td>-0.009</td>
<td>32</td>
</tr>
<tr>
<td>SG-3</td>
<td>27.1</td>
<td>0.010</td>
<td>38</td>
</tr>
<tr>
<td>2400</td>
<td>28.3</td>
<td>0.017</td>
<td>34</td>
</tr>
<tr>
<td>2385</td>
<td>24.8</td>
<td>0.029</td>
<td>36</td>
</tr>
<tr>
<td>2360</td>
<td>19.2</td>
<td>0.032</td>
<td>34</td>
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<tr>
<td>2330</td>
<td>29.8</td>
<td>0.007</td>
<td>33</td>
</tr>
<tr>
<td>2253</td>
<td>26.6</td>
<td>0.014</td>
<td>36</td>
</tr>
<tr>
<td>1886</td>
<td>39.3</td>
<td>0.006</td>
<td>44</td>
</tr>
<tr>
<td>1800</td>
<td>38.2</td>
<td>0.008</td>
<td>43</td>
</tr>
<tr>
<td>3359</td>
<td>32.2</td>
<td>0.006</td>
<td>37</td>
</tr>
<tr>
<td>3356</td>
<td>28.9</td>
<td>0.013</td>
<td>38</td>
</tr>
<tr>
<td>3209</td>
<td>32.9</td>
<td>0.006</td>
<td>38</td>
</tr>
<tr>
<td>3200</td>
<td>28.9</td>
<td>0.010</td>
<td>35</td>
</tr>
<tr>
<td>2915</td>
<td>30.0</td>
<td>0.016</td>
<td>39</td>
</tr>
<tr>
<td>1789</td>
<td>30.9</td>
<td>0.013</td>
<td>35</td>
</tr>
</tbody>
</table>

Tab. 2.4: Coefficients of the linear regressions \(q(z) = A + Bz\) plotted in figure 2.16. Specific heat flow values from table 2.2 are given for comparison.
2.4 Results and discussion of numerical simulations

In order to study and quantify the effects responsible for the vertical variation in specific heat flow, it is necessary to perform 3-D numerical simulations of heat transport and fluid flow. As a follow-up and extension of previous work in Kukkonen and Clauser (1994), a regional 3-D model was set up, aligned along the direction of the synclinal structure, extending from some distance south-west of the super-deep borehole (the local water divide) to the north-east towards the Barents Sea (figure 2.17). Its dimensions are 20 km × 60 km × 15 km. Figure 2.17 shows the location of the model area, its size, as well as the seven main lithological units. Their main thermal and physical properties are listed in Tab. 2.6. A 3-D finite difference code is used for the numerical simulation of heat and mass flow (see 1.2.1). Additionally, because of the northern location of the study area, latent heat effects due to freezing and thawing of subsurface fluids were implemented in the code. Table 2.7 summarises the main properties of the numerical model. On

<table>
<thead>
<tr>
<th>Rock</th>
<th>Shallow boreholes</th>
<th>SG-3 borehole</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \lambda_{\text{eff}} ) (W m(^{-1}) K(^{-1}))</td>
<td>( \lambda_{\text{par}} ) (W m(^{-1}) K(^{-1}))</td>
</tr>
<tr>
<td></td>
<td>Average RMS N</td>
<td>Average RMS N</td>
</tr>
<tr>
<td>Diabase (effusive)</td>
<td>2.97</td>
<td>3.28</td>
</tr>
<tr>
<td></td>
<td>2.05-4.41</td>
<td>2.56-4.30</td>
</tr>
<tr>
<td></td>
<td>0.44</td>
<td>0.41</td>
</tr>
<tr>
<td></td>
<td>162</td>
<td>162</td>
</tr>
<tr>
<td>Tuff, Tuffite</td>
<td>3.44</td>
<td>3.83</td>
</tr>
<tr>
<td></td>
<td>2.36-5.47</td>
<td>2.75-5.54</td>
</tr>
<tr>
<td></td>
<td>0.61</td>
<td>0.67</td>
</tr>
<tr>
<td></td>
<td>141</td>
<td>141</td>
</tr>
<tr>
<td>Rhythmic layered sandstone,</td>
<td>3.63</td>
<td>3.77</td>
</tr>
<tr>
<td>siltstone, phylite</td>
<td>1.29-7.11</td>
<td>2.64-6.27</td>
</tr>
<tr>
<td></td>
<td>0.67</td>
<td>0.55</td>
</tr>
<tr>
<td>Nickel-bearing intrusion gabbro,</td>
<td>2.93</td>
<td>2.88</td>
</tr>
<tr>
<td>pyroxene, peridot</td>
<td>2.12-6.07</td>
<td>2.20-3.88</td>
</tr>
<tr>
<td></td>
<td>0.58</td>
<td>0.4</td>
</tr>
<tr>
<td></td>
<td>246</td>
<td>246</td>
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<tr>
<td>gabbro-diabase (intrusion)</td>
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<td>3.45</td>
</tr>
<tr>
<td></td>
<td>2.26-6.41</td>
<td>2.79-4.13</td>
</tr>
<tr>
<td></td>
<td>0.47</td>
<td>0.43</td>
</tr>
<tr>
<td></td>
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<tr>
<td>actinolite diabase</td>
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<td>3.45</td>
</tr>
<tr>
<td></td>
<td>2.78-4.30</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>0.44</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>18</td>
<td>18</td>
</tr>
<tr>
<td>gneiss</td>
<td>2.94</td>
<td>2.99</td>
</tr>
<tr>
<td></td>
<td>1.82-5.55</td>
<td>2.17-3.70</td>
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<tr>
<td></td>
<td>0.58</td>
<td>0.34</td>
</tr>
<tr>
<td></td>
<td>42</td>
<td>42</td>
</tr>
<tr>
<td>amphibolite</td>
<td>2.52</td>
<td>2.88</td>
</tr>
<tr>
<td></td>
<td>1.79-3.44</td>
<td>2.55-3.43</td>
</tr>
<tr>
<td></td>
<td>0.41</td>
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<td></td>
<td>16</td>
<td>16</td>
</tr>
</tbody>
</table>

Tab. 2.5: Results of thermal conductivity measurements for shallow boreholes and the Kola super-deep borehole. N is the number of samples studied.
2. Heat transport processes in the upper crust near the Kola super-deep borehole

Fig. 2.17: 3D Model of the Kola area. Numbers indicate the different lithological units described in Tab. 2.6.

<table>
<thead>
<tr>
<th>Rock Type</th>
<th>Code</th>
<th>Color</th>
<th>( \lambda ) (W m(^{-1})K(^{-1}))</th>
<th>( A ) (W m(^{-2}))</th>
<th>( \rho c_p ) (MJ m(^{-3})K(^{-1}))</th>
<th>( \phi ) (-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basic magmatic rocks</td>
<td>1</td>
<td>blue</td>
<td>3.0 ±0.4</td>
<td>0.67</td>
<td>2.06</td>
<td>0.007</td>
</tr>
<tr>
<td>Metasedimentary rocks</td>
<td>2</td>
<td>light blue</td>
<td>3.3 ±0.8</td>
<td>0.26</td>
<td>2.06</td>
<td>0.001</td>
</tr>
<tr>
<td>Volcanic rocks</td>
<td>3</td>
<td>dark green</td>
<td>3.4 ±0.7</td>
<td>0.4</td>
<td>2.06</td>
<td>0.02</td>
</tr>
<tr>
<td>Diabase</td>
<td>4</td>
<td>light green</td>
<td>3.0 ±0.6</td>
<td>0.56</td>
<td>2.06</td>
<td>0.018</td>
</tr>
<tr>
<td>Gneiss 1</td>
<td>5</td>
<td>yellow</td>
<td>2.9 ±0.5</td>
<td>1.4</td>
<td>2.06</td>
<td>0.01</td>
</tr>
<tr>
<td>Gneiss 2</td>
<td>6</td>
<td>orange</td>
<td>2.6 ±0.4</td>
<td>1.47</td>
<td>2.06</td>
<td>0.008</td>
</tr>
<tr>
<td>Gneiss/Granitoid</td>
<td>7</td>
<td>red</td>
<td>2.9 ±0.5</td>
<td>0.6</td>
<td>2.06</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Tab. 2.6: Thermal and physical parameters of the 3D model. Data taken from Kukkonen and Clauser (1994), Popov et al. (1999b) and this study.

the surface a mean annual temperature is assumed, which varies adiabatically with topography from about 1 °C – 4 °C. Due to the prevailing uniform precipitation (500 mm – 700 mm per year), the hydraulic head is identified with elevation. In figure 2.17 the structure on the model’s surface reflects the topography of the area.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh Size:Resolution</td>
<td>116 m × 35 m × 100 m; 512 m × 512 m × 100 m</td>
</tr>
<tr>
<td>Basal heat flow ( q )</td>
<td>40 mW m(^{-2})</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>( f(T) )</td>
</tr>
<tr>
<td>Thermal capacity</td>
<td>( f(T) )</td>
</tr>
<tr>
<td>Geological Units</td>
<td>7</td>
</tr>
<tr>
<td>Thermal boundary conditions</td>
<td>On the surface: const T, bottom: constant q</td>
</tr>
<tr>
<td>Hydraulic boundary conditions</td>
<td>On the surface: constant head, else: no flow</td>
</tr>
</tbody>
</table>

Tab. 2.7: Properties and boundary conditions of the 3-D model. The variation of thermal conductivity and capacity with temperature of the different rock types is taken from this study.
2.4. Results and discussion of numerical simulations

Fig. 2.18: Results of the steady-state conductive and advective heat transfer simulations, compared to data from the literature. Left: Temperature-depth profile from data and modelling in the SG-3. In the upper 2 km the data from Popov et al. (1999b) is not sufficiently resolved as shown by the comparison with a shallow hole (Nr. 3200) near the SG-3. Right: Variation of specific heat flow (vertical component) in the SG-3 with depth from data and modelling for different model runs, discussion see text.

2.4.1 Advection and heterogeneity: steady-state simulations

Figure 2.18 shows a comparison of the simulated steady-state temperature- and heat flow-depth profile with existing data from the super-deep borehole SG-3 (Popov et al. 1999b; Borevsky et al. 1995). Since the resolution of the temperature in the upper 2 km from data in Popov et al. (1999b) is not sufficient, the inset illustrates the good agreement of the model’s output with data presented in this study, a temperature log of borehole 3200, located less than 1 km away from the SG-3. The more recent specific heat flow data are systematically higher. This trend is confirmed by the calculations, especially in the upper 5 km. Down to a depth of 4 km the purely conductive model deviates significantly from the data. The increase of specific heat flow is about 30 mW m\(^{-2}\) within this depth range, which cannot be explained by a purely conductive model. This implies a strong dependence on permeability. However, since information on permeability in the study area is poor, a simplified, horizontally layered model for permeability is applied according to Borevsky et al. (1987) and from information obtained during the field campaign in 1994.
Heat transport processes in the upper crust near the Kola super-deep borehole

<table>
<thead>
<tr>
<th>Depth range (m)</th>
<th>Permeability (m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 – 2000</td>
<td>3·10⁻¹⁶</td>
</tr>
<tr>
<td>2000 – 4000</td>
<td>4·10⁻¹⁵</td>
</tr>
<tr>
<td>4000 – 6000</td>
<td>1·10⁻¹⁶</td>
</tr>
<tr>
<td>6000 – 8000</td>
<td>1·10⁻¹⁷</td>
</tr>
<tr>
<td>8000 – 10000</td>
<td>1·10⁻¹₈</td>
</tr>
<tr>
<td>10000 – 12000</td>
<td>1·10⁻¹₉</td>
</tr>
<tr>
<td>12000 – 14000</td>
<td>1·10⁻₂₀</td>
</tr>
<tr>
<td>14000 – 15000</td>
<td>1·10⁻₂₁</td>
</tr>
</tbody>
</table>

Tab. 2.8: Horizontally layered model for permeability (after Borevsky et al. (1987) and Clauser et al. (1999)).

Additionally, it is assumed that this simplified permeability distribution extends throughout the model. Being aware that this information is very vague, more data were not available for this study. In the light of this limitation, some general aspects of permeability in the upper crystalline crust need to be considered. In contrast to sedimentary regimes, permeability is controlled by fractures. Therefore, it is an approximation to consider the rock as a homogenous porous medium (Kukkonen, 1995).

Manning and Ingebritsen (1999) discuss the permeability of the Earth’s crust in general. By simplified analysis of models and data, neglecting the issues of heterogeneity, time, and scale dependence of permeability, they obtain typical values of permeability from 10⁻¹⁷ m² to 10⁻¹⁴ m², with a mean value around 10⁻¹⁶ m². Data from Clauser (1992) is consistent with these values. Permeability adapted for the model is located within a similar range to a depth of 8 km (table 2.8). Below 8 km there is practically no flow in the model due to the very low permeability values. This can also be seen in figure 2.18.

Manning and Ingebritsen (1999) also suggest a general, quasi-exponential decay of permeability with depth \( z \) of \( \log k \approx -3.2 \log z - 14 \) due to loss of porosity through depth-increasing confining pressure. Figure 2.19 shows the comparison of this relation with the values adapted here. Whereas in the upper 8 km the values from this study scatter around the general curve, they are much lower in the deeper parts. However, the interesting depth range is above that depth where flow might be important (figure 2.18). The general relation by Manning and Ingebritsen (1999) is also considered in the model (see below).

The sharp increase in specific heat flow at a depth of about 4.8 km results from a few measured high values of thermal conductivity. In the model the average conductivity of the corresponding unit 3, however, is considerably lower, although it includes these few high values (see figure 2.17). Thus, this peak cannot be reproduced by the model. In the deeper part of the SG-3 (below 5 km), the simulated specific heat flow is systematically lower. This deviation is most probably due to some uncertainty regarding the pressure dependence of thermal conductivity which is accounted for in the data from Popov et al. (1999b), but not yet in the model. In contrast to the decrease of thermal conductivity with temperature, there is an increase with pressure which can be on the order of 20 % (Clauser and Huenges, 1995). This aspect requires more sensitivity studies in order to find a suitable relation between thermal conductivity and pressure.

To illustrate the influence of varying thermal conductivity, figure 2.18 also shows how results differ when thermal conductivity is kept either constant or when it varies within the standard deviation. This variation only yields a difference of a few mW m⁻² in specific heat flow, decreasing with depth. In order to visualise the effect of the inclined layers of the Pechenga structure (figure 2.17) on the different tensor components of heat flow, in figure 2.20 the relative contribution of the vertical component of heat flow, \( q_z \), and the horizontal component, \( q_{xy} = \sqrt{q_x^2 + q_y^2} \), is shown. Although the structure of the inclined layers becomes...
visible, the vertical component dominates the specific heat flow with a relative contribution greater than 95%, except some surface effects, but which are probably of a numerical nature. Thus, the refraction of heat flow does not play a significant role.

Another effect which might affect the steady state advective model is the fluid’s salinity. Borevsky et al. (1987) and Kremenetsky and Ovchinnikov (1986) provide data on salinity in the Kola area. In general, the groundwater is fresh and isotopically meteoric in composition to about 1 km level, below which saline fluids and even brines of Ca-Na-Cl composition of 100 mg L$^{-1}$ to 300 mg L$^{-1}$ control the hydrogeochemistry. However, substituting the fresh water by these brines in the model did not cause any significant changes in the results.

Results of these steady-state simulations imply that heterogeneity is less important and advection is the main reason for the increase of specific heat flow with depth in the upper 4 km. Figure 2.21 show a vertical section of the steady state coupled model, using permeability data from table 2.8. At the super-deep borehole, heat is transferred by advection downwards, whereas in the topographic lows the fluid flow is directed upwards, yielding higher specific heat flow values. The sparse information on permeability requires a sensitivity analysis, however. Therefore, in additional model runs permeability was increased and decreased, respectively, by an order of magnitude compared to those in table 2.8. The result is shown in figure 2.22. Obviously the data in table 2.8 is the range where the transition between a conductively and advectively dominated regime. This is in agreement with Manning and Ingebritsen (1999) who state that significant advective heat transport typically requires permeabilities greater than $10^{-16}$ m$^2$. The quasi-exponential model differs somewhat from the local model, suggesting that in the upper part permeabilities are overestimated. Taking these facts into account, from mere steady-state simulations, the increase of

**Fig. 2.19:** The quasi-exponential decay (black line) of permeability $k$ with depth in the upper crust (Manning and Ingebritsen, 1999) in comparison with permeability from Borevsky et al. (1987) and Clauser et al. (1999) (grey circles).
Fig. 2.20: Relative contribution of vertical \((q_z)\) and horizontal \((q_{xy})\) components of specific heat flow. Panel (a) shows the vertical section including the super-deep borehole in x-direction (figure 2.17) and (b) the section in y-direction.
2.4. Results and discussion of numerical simulations

![Graph showing thermal and flow characteristics](image)

**Fig. 2.21:** Vertical component $q_z$ of specific heat flow and Darcy-velocity $v_D$, extracted from the 3-D steady-state, coupled model.

![Graph comparing simulations and literature data](image)

**Fig. 2.22:** Results of the steady-state simulations, compared to data from the literature and different permeabilities. The variation of specific heat flow with depth strongly depends on permeability. Discussion see text.
specific heat flow with depth cannot be attributed to advection definitely.

2.4.2 Palaeoclimate: transient forward simulations

For simulating the transient behaviour of the subsurface thermal regime by forward calculations, a very simple boxcar model is applied representing the temperature change from the Late Pleistocene to the Holocene in three different magnitudes (see inset in figure 2.23). At 80 ky BP the temperature drops from 1 °C to -14 °C, -8 °C, and -4 °C, respectively, and rises again to the initial value at 15 ky BP. The first case, the rather large step, is likely to be an exaggeration and therefore yields an upper limit of the palaeoclimatic effect. The initial condition for this transient modelling are provided by the steady-state model (see above). As illustrated in figure 2.23, two different scenarios are considered: The purely conductive model satisfies the data worst, although it does show an increase in specific heat flow in the top 2.5 km which is not reproduced at all by the purely conductive steady-state calculations. For the case of the smaller temperature changes (ΔT=5 K and ΔT=9 K), the effect becomes obviously smaller. As expected, the coupled model (heat and flow transport) explains the increase in specific heat flow much better. For comparison, the result of the steady-state coupled model is plotted together with the transient simulation. The latter one shows a slightly larger increase in specific heat flow, satisfying the data just below 2 km depth better. Again, there is a deviation between data and model below 5 km where palaeoclimatic disturbances vanish. This may be an indication that the variation of thermal conductivity with pressure is not adequately accounted for.

In order to find a better constraint for the magnitude of the temperature increase from the Pleistocene to the Holocene, joint inversions were performed taking advantage of the several temperature logs available from the shallow holes (see Chapter 3). These results imply higher temperatures during the Pleistocene than assumed in the forward calculations, since the temperature change is on the order of 4 K – 7 K rather than 9 K or even 15 K. This is probably due to an insulating effect of the ice cover which has prevailed for long times during the Pleistocene (Siegert et al. 2001). This results in smaller temperature changes than observed in lower latitudes, i.e. 7 K – 11 K in the Czech republic (ˇSafanda and Rajver 2001) or southeast Germany (Clauser et al. 1997).

As a conclusion, the increase in specific heat flow can be attributed neither totally to advection nor to palaeoclimate. Heterogeneity is less important. The steady-state simulations show that in the case of the Kola super-deep borehole the increase in specific heat flow from about 30 mW m⁻² – 60 mW m⁻² is mainly due to advection, and caused by the topographically driven flow. However, these results are based on a simplified model of permeability.

In order to better quantify the influences of the different processes a detailed, larger scaled model would be necessary. However, due to the lack of further geophysical logs besides temperature and thermal conductivity, detailed sensitivity analysis is required. This study is in preparation (Mottaghy and Rath 2007).

Nevertheless, purely conductive transient simulations show that the influence of palaeoclimatic changes in surface temperatures cannot be neglected, because they yield a variation in specific heat flow of more than half of the observed magnitude in this case. However, it is likely to be less because of the higher temperatures during the late Pleistocene. Nevertheless, regarding vertical increase in specific heat flow with depth in other deep boreholes, no general statement can be made. In fact, the local conditions (topography,
Fig. 2.23: Results of the transient simulations, compared to data from the literature. Left: Temperature-depth profile from data and modelling SG-3. The inset illustrates the boxcar model representing a simplified model of the palaeoclimate for the last 80 kY. Right: Variation of specific heat flow (vertical component) in the SG-3 with depth from data and modelling, discussion see text.
palaeoclimate, and ice cover) determine which process dominates and may be held responsible for this variation. This conclusion is in agreement with the general result of Kukkonen and Jöeleht (2003), who observe a common increase of heat flow in a compilation of a large data set of the Fennoscanian Shield and the Eastern European Platform regardless of hydrological systems. This and the findings here both suggest that both palaeoclimate and heat advection may contribute to this effect. Therefore, both effects need to be studied in combination. In particular, this requires a detailed study of the correlation between borehole altitudes and the magnitude of the vertical variation in specific heat flow. A first indication is provided by the vertical profile of specific heat flow in borehole 3396, which is based on a temperature log obtained during this study. It is situated 50 km south of the super-deep borehole and is thus not located in the elevated terrain of the Pechenga structure (figure 2.11). Here, advection will not be important, and, indeed, no vertical increase in specific heat flow is observed (figure 2.16, uppermost profile).
3. PALAEOTEMPERATURE RECONSTRUCTIONS FOR THE KOLA PENINSULA AND NORTHERN POLAND

The inversion technique introduced in section 1.2.2 is applied in this chapter for the reconstruction of palaeotemperatures in two different areas: on the Kola Peninsula, using the data set presented in the previous chapter, and in northeastern Poland, using data from a deep borehole. It is shown that in the high porosity environment of the Polish borehole, it is essential to account for the latent heat effects which are briefly described in section 1.1.4. Therefore, the first part of this chapter gives a deeper discussion of implementing and verifying the latent heat effects in the forward and the inverse code. The second part focuses on the palaeotemperature reconstructions for both study areas. The chapter is published in Mottaghy and Rath (2006), and additionally parts of it in Mottaghy and Rath (2007).

3.1 The latent heat effect: Numerical methods

In the following, a simple but effective method is described for modelling of freezing and thawing processes in the subsurface. The so called enthalpy method has been used by several authors before (e.g. Galushkin, 1997; Lunardini, 1987). This scheme has been implemented into the forward modelling code SHEMAT, as well as the inverse code, both presented in chapter 1.

3.1.1 Frozen soil physics

When modelling the thermal effects of freezing and thawing, obviously equation (1.17) has to include three phases: matrix, fluid, and ice. To achieve this, the following volume fractions are defined:

$$\phi_m = 1 - \phi, \phi_f = \phi \cdot \Theta, \phi_i = \phi - \phi_f,$$

(3.1)

where $\Theta$ denotes the fraction of pore space occupied by fluid, and an additional ice phase is introduced marked by index $i$. The constraint $\phi_m + \phi_i + \phi_f = 1$ implies that pore space is completely saturated.

As a result of the complicated processes in the porous medium, thawing can not be considered as a simple discontinuity. $\Theta$ is generally assumed to be a continuous function of temperature in a specified interval (Lunardini, 1987), e.g.,

$$\Theta = \begin{cases} 
\exp[-\left(\frac{T-T_L}{w}\right)^2] & \text{if } T < T_L \\
1 & \text{if } T > T_L
\end{cases}$$

(3.2)

This function is shown in figure 3.1. It is characterised by a thawing temperature $T_L$ (liquidus, usually 0 °C) and a parameter $w$ (usually $\geq 1$ K). If $w$ is set to 1, it corresponds to a freezing interval $\Delta T = T_L - T_S \approx 2K$, where $T_S$ is the freezing temperature (solidus), at which almost all fluid is frozen (dotted...
Fig. 3.1: Smooth partition function $\Theta$ (left) and its derivative with respect to $T$ (right) according to equations (3.2) and (3.8) for several values of the thawing interval $w$. The area below the curves in the figure on the right are equal, which satisfies the latent heat condition equation (3.9).

Fig. 3.2: Freezing of soil: an example for a non isothermal cooling curve due to latent heat, as opposed to instantaneous freezing. The curves show the temperature at 50 cm depth in a homogenous porous medium ($\phi=0.4$, $\lambda=2.5$ W m$^{-1}$ K$^{-1}$). Here, $T_S = -2.5\, ^\circ C$.

line in figure 3.1. However, this range is a user specified parameter, making it possible to analyse a variety of ground conditions. Figure 3.2 shows an example for the variation of the temperature with time. Here, the surface is exposed to a fixed temperature of -3 $^\circ$C, resulting in a cooling of the soil below the initial temperature of 0 $^\circ$C. As the freezing occurs within the temperature range $T_L - T_S$ the phase transition is not adiabatic.

3.1.2 Apparent heat capacity

Usually the concept of an apparent or effective heat capacity is invoked in order to account for the latent heat associated with thawing and freezing by expanding the term considering matrix and fluid on the right-
The latent heat effect: Numerical methods

The contribution by fluid and ice, subscript f and i, respectively, can be expressed as the derivative of fluid enthalpy \( H_f \) with respect to time. During thawing, this fluid enthalpy per unit volume changes according to

\[
\Delta H_f = \int (\phi_f \rho_f c_f + \phi_i \rho_i c_i) \, dT - \int \rho_i L \, d\phi_i ,
\]

(3.3)

where \( \phi_f \) and \( \phi_i \) are the relative volumes occupied by free and frozen fluid, respectively. \( L \) is the specific latent heat (for water \( \approx 333.6 \, \text{kJ kg}^{-1} \)). Obviously, a volumetric apparent specific heat capacity \((\rho c)_a\) can be defined, which includes additional energy sources or sinks due to latent heat and replaces the fluid contribution of the term in parentheses on the right hand side of equation (1.17):

\[
(\rho c)_a = \phi_f \rho_f c_f + \phi_i \rho_i c_i - \frac{\rho_i L}{d\phi_i} .
\]

(3.4)

The total derivative in the last term of equation (3.4) is usually approximated by finite differences, resulting in a constant apparent specific heat \( L' \):

\[
L \frac{\Delta \phi_i}{\Delta T} = L \frac{\phi_{i,L} - \phi_{i,S}}{\Delta T} = L' \frac{\Delta T}{\Delta T} .
\]

(3.5)

where \( \phi_{i,L} \) and \( \phi_{i,S} \) are the volume fractions at liquidus and solidus temperatures, respectively. The freezing range is thus described by the temperature interval \( \Delta T = T_L - T_S \) with fixed temperatures \( T_S \) and \( T_L \) at which all of the fluid is frozen or unfrozen, respectively (see section 3.1.1). This choice leads to an apparent heat capacity of

\[
(\rho c)_a = \begin{cases} 
\phi_f \rho_f c_f & T > T_L \\
\phi_f \rho_f c_f + \phi_i \rho_i c_i - \frac{\rho_i L}{d\phi_i} & T_S \leq T \leq T_L \\
\phi_i \rho_i c_i & T \leq T_S,
\end{cases}
\]

(3.6)

with

\[
\Delta T = \begin{cases} 
T_L - T_S & \text{when thawing} \\
T_L - T_S & \text{when freezing}.
\end{cases}
\]

(3.7)

In equation (3.6), \( \rho \) and \( c \) are functions of temperature. For the fully unfrozen state the variation with temperature of these are as described in Clauer (2003) and for the fully frozen state properties of ice at different temperatures are taken from Miller (1982) and Lide (2000). Table 3.1 lists some values for water and ice for comparison. Figure 3.3 illustrates, how \((\rho c)_a\) varies with temperature. This approximation of a constant apparent heat capacity is consistent with assuming a step function for \( \Theta \). Since a smoother function is used (equation (3.2)), it can be simply differentiated:

\[
\frac{d\Theta}{dT} = \begin{cases} 
-2 \frac{(T - T_L)}{w^2} \exp \left[ - \left( \frac{T - T_L}{w} \right)^2 \right] & \text{if } T \leq T_L \\
0 & \text{if } T > T_L.
\end{cases}
\]

(3.8)

This can be used in equations (3.1) and (3.4) instead of the approximation in equation (3.5). The function \( \Theta \) and its derivative are shown in figure 3.1.

According to Bonacina and Comini (1973) the actual shape of this curve is not important with regard to
3. Palaeotemperature reconstructions for the Kola peninsula and Northern Poland

**Fig. 3.3:** Apparent heat capacity \((\rho c)_a\) as a function of temperature below or above the solidus or liquidus temperature \(T_L - T_S\), respectively. \(\Theta\) is assumed as a ramp function, leading to a piecewise constant \((\rho c)_a\).

<table>
<thead>
<tr>
<th>(T) (°C)</th>
<th>(\rho) (kg m(^{-3}))</th>
<th>(c_p) (kJ kg(^{-1}) K(^{-1}))</th>
<th>(\lambda) (W m(^{-1}) K(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>916.7</td>
<td>2.11</td>
<td>2.14</td>
</tr>
<tr>
<td>-10</td>
<td>918.7</td>
<td>2.03</td>
<td>2.30</td>
</tr>
<tr>
<td>-20</td>
<td>920.3</td>
<td>1.96</td>
<td>2.40</td>
</tr>
<tr>
<td>-30</td>
<td>921.6</td>
<td>1.88</td>
<td>2.50</td>
</tr>
<tr>
<td>-40</td>
<td>922.8</td>
<td>1.80</td>
<td>2.60</td>
</tr>
</tbody>
</table>

**Tab. 3.1:** Temperature, density, specific heat capacity, and thermal conductivity of ice at some temperatures (from Miller [1982]).

Although no underlying physical meaning can be given, this mixing law has mathematical analogies with calculations of dielectrical permittivity and electrical conductivity (Cosenza et al., 2003). Values for the
properties of ice are taken from \cite{Miller1982}. Note that other mixing laws may be employed, leading to an corresponding change in equations \ref{eq:3.14} and \ref{eq:3.15}.

\section*{3.2 Model verification}

In order to verify the approach described above, the solutions are compared to a very special case where an analytical solution exists as well as to a more general cases, using other numerical models. Both models are purely conductive.

\subsection*{3.2.1 Analytical solution}

The solutions to conductive heat transfer problems with solidification phase change and the release or consumption of latent heat – often referred to as "Stefan problems" \cite{Stefan1891} – are inherently non-linear and thus, solution methods are very restricted. A classical solution for a semi-infinite medium with constant temperature undergoing a step change of surface temperature was given by \citeauthor{NeumannCa.1860} (ca. 1860) and has been expanded by \citeauthor{CarslawJaeger1959} \citeyear{CarslawJaeger1959}. It is called the Neumann solution and specifies the location \( X(t) \) of the phase front (i.e. the isotherm \( T = T_S \)) as a function of time. A liquid is at \( T = T_L \) for \( x > 0 \). At time \( t = 0 \) the surface \( x = 0 \) is exposed to a temperature \( T_0 \) lower than \( T_S \). The phase front \( X \), i.e. the isotherm \( T = T_S \) is moving with time as (see figure 3.4)

\[
X(t) = 2\gamma \sqrt{\kappa_i t} .
\tag{3.11}
\]

Here and in equation \ref{eq:3.12}, \( \kappa_i \) and \( \kappa_f \) indicates the thermal diffusivity of ice and water, respectively. The parameter \( \gamma \) must be determined from the following equation \cite{CarslawJaeger1959} that results from the boundary conditions of the associated differential equation (with the thermal conductivities \( \lambda_{i,f} \) of both materials):

\[
\frac{\exp[(\kappa_i - \kappa_f)\gamma^2/\kappa_f]}{\text{erf} \gamma} \text{erf} \gamma \left[ \gamma \sqrt{\kappa_i/\kappa_f} \right] - \frac{(T_L - T_S)\lambda_f \sqrt{\kappa_i}}{(T_S - T_0)\lambda_i \sqrt{\kappa_f}} .
\tag{3.12}
\]

The latent heat effect is considered approximately in equation \ref{eq:3.12} by adding the expression of equation \ref{eq:3.5} to the thermal diffusivity of the liquid:

\[
\kappa_f = \frac{\lambda_f}{\rho_f c_f + \frac{L}{\Delta T}} .
\tag{3.13}
\]

Equation \ref{eq:3.11} is solved for \( \gamma \) by an in built function of MATLAB® which uses a numerical algorithm to determine the roots. Table \ref{tab:3.2} lists some computed values of \( \gamma \) for several values of the temperature difference \( \Delta T \).

\subsection*{Model properties}

A horizontal domain of 20 \times 100 nodes and a mesh size of 1 cm is chosen as an approximation for the semi-infinite half-space. The model is purely conductive. Since the analytical solution \ref{eq:3.11} is strictly valid only for a homogeneous fluid, the porosity must be chosen as large as possible. Here, in a first
Tab. 3.2: The parameter $\gamma$ for different widths of freezing range $\Delta T$.

<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>$\Delta T$ (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.039</td>
<td>4</td>
</tr>
<tr>
<td>0.041</td>
<td>3</td>
</tr>
<tr>
<td>0.043</td>
<td>2</td>
</tr>
</tbody>
</table>

Fig. 3.4: The Neumann problem: Location $X(t)$ of the phase front $T=T_S$. 
3.2. Model verification

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid size; Resolution</td>
<td>20 x 100; 1 cm</td>
</tr>
<tr>
<td>Temperature</td>
<td>0 °C (-3 °C at x=0)</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.95 and 0.05</td>
</tr>
<tr>
<td>Matrix thermal capacity</td>
<td>2.06 MJ m⁻³ K⁻¹</td>
</tr>
<tr>
<td>Matrix thermal conductivity</td>
<td>2.9 W m⁻¹ K⁻¹</td>
</tr>
<tr>
<td>Time step size; Total Simulation time</td>
<td>864 s; 100 days and 1.8 days</td>
</tr>
</tbody>
</table>

Table 3.3: Model parameters used in the verification problem.

<table>
<thead>
<tr>
<th>Time (d)</th>
<th>$X_{ana}$ (cm)</th>
<th>$X_{num}$ (cm)</th>
<th>% Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>5.4</td>
<td>6</td>
<td>10</td>
</tr>
<tr>
<td>20</td>
<td>12.6</td>
<td>13</td>
<td>3.5</td>
</tr>
<tr>
<td>50</td>
<td>19.6</td>
<td>20</td>
<td>2.2</td>
</tr>
<tr>
<td>80</td>
<td>24.6</td>
<td>25</td>
<td>1.5</td>
</tr>
<tr>
<td>99</td>
<td>26.9</td>
<td>27</td>
<td>0.035</td>
</tr>
</tbody>
</table>

Table 3.4: Location $X(t)$ of the isotherm $T = T_S$ at different times for $\phi = 0.95$ obtained from the analytical (ana) and numerical (num) solutions.

approximation, a value of 0.95 is chosen. Later, a more realistic porosity of 0.05 will be used which requires a modification of the analytical solution. The initial temperature of the half-space is the warm end of the freezing range ($T_L = 0$ °C). At $t = 0$, the surface at $x = 0$ is exposed to a temperature of $T_0 = -3$ °C $< T_S$. The other parameters are summarised in table 3.3.

Results and discussion

Figure 3.5 shows the propagation of the phase front $X(t)$. In the beginning, the numerical solution (crosses) overestimates the location of the freezing front, but the error decreases with time, becoming less than 5 % after ten days. At longer times, the difference between analytical and numerical solution vanishes even more. The initially significant deviation is due to the coarse discretisation of the grid and boundary effects. The influence of both factors decreases as the phase front propagates. They error decreases also for smaller time steps. Additional error sources arise from the fact that a porosity of 1.0 cannot be simulated in SHEMAT and the approximation inherent in the choice of the function $\Theta$ shown in figure 3.1. Table 3.4 lists some values of the analytical and numerical solution, as well as the percentage deviation.

Next, the heterogeneous soil structure is taken into account. The thermal conductivity is weighted by the square-root mean (see section 3.1.3) and the the thermal capacity by the arithmetic mean. Since the properties in equation (3.12) refer only to the fully unfrozen (f) or the fully frozen (i) state, it is sufficient to use the porosity $\phi$ as in equation (1.17). Thus, the thermal diffusivity of the fluid becomes from equation (3.12)

$$\kappa_f \rightarrow \kappa_{f,m} = \frac{(\phi \sqrt{\lambda_f} + (1-\phi) \sqrt{\lambda_m})^2}{\phi \rho_f c_f + (1-\phi) \rho_m c_m + \frac{\rho_f L}{\Delta T}}.$$ (3.14)
3. Palaeotemperature reconstructions for the Kola peninsula and Northern Poland

![Graph showing freezing front propagation over time for numerical and analytical solutions.]

**Fig. 3.5:** Propagation of the phase front $X(t)$ for the Neumann problem and a porosity $\phi = 0.95$.

<table>
<thead>
<tr>
<th>Time (h)</th>
<th>$X_{ana}$ (cm)</th>
<th>$X_{num}$ (cm)</th>
<th>% Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>5.9</td>
<td>6</td>
<td>1.5</td>
</tr>
<tr>
<td>18</td>
<td>8.9</td>
<td>9</td>
<td>1.4</td>
</tr>
<tr>
<td>22</td>
<td>9.9</td>
<td>10</td>
<td>1.4</td>
</tr>
<tr>
<td>27</td>
<td>10.9</td>
<td>11</td>
<td>1.4</td>
</tr>
<tr>
<td>32</td>
<td>11.8</td>
<td>12</td>
<td>1.4</td>
</tr>
</tbody>
</table>

**Tab. 3.5:** Location $X(t)$ of the isotherm $T = T_s$ at different times for $\phi = 0.05$ obtained from the analytical (ana) and numerical (num) solutions.

And the thermal diffusivity of ice becomes

$$\kappa_i \rightarrow \kappa_{i,m} = \frac{(\phi \sqrt{\lambda_i} + (1 - \phi) \sqrt{\lambda_m})^2}{\phi \rho_i c_w (1 - \phi) \rho_m c_m}.$$  \hspace{1cm} (3.15)

Figure 3.6 shows the evolution of the phase front for a porosity of 0.05 using the modified analytical solution compared to the previous case ($\phi=0.95$). The front propagates faster, because due to the lower water content less latent heat is released. Table 3.5 lists some values of the analytical and numerical solution for comparison.

### 3.2.2 Comparison with numerical models

The model is compared to an existing software, GeoStudio™ by GEO-SLOPE International. The module TEMP/W described in [GEO-SLOPE™ (2004)] is developed for finite element geothermal analysis. It includes Neumann thawing and freezing analysis for which a similar verification example is given as that presented in section 3.2. Table 3.6 illustrates the selected parameters for the verification example for TEMP/W. The volumetric water content is idealised and set to 1. The analytical solution assumes a single temperature step for the phase change at 0 °C. Since this numerically critical, TEMP/W uses a near-perfect step function: Within a range of 1 mK below 0 °C the volumetric water content changes.
3.2. Model verification

Figure 3.6: Propagation of the phase front $X(t)$ for the Neumann problem and a porosity $\phi = 0.05$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid size; Resolution</td>
<td>10 x 500; 1 cm</td>
</tr>
<tr>
<td>Ground temperature</td>
<td>-3 °C</td>
</tr>
<tr>
<td>Surface temperature</td>
<td>5 °C</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.99</td>
</tr>
<tr>
<td>Matrix thermal capacity</td>
<td>2.0 MJ m$^{-3}$K$^{-1}$</td>
</tr>
<tr>
<td>Matrix thermal conductivity</td>
<td>1.15 W m$^{-1}$K$^{-1}$</td>
</tr>
<tr>
<td>Total Simulation time</td>
<td>1200 d</td>
</tr>
</tbody>
</table>

Tab. 3.6: Parameters of the verification example adapted from TEMP/W.

from 1 to 0. In contrast, this model features a freezing interval from 0 °C to -2 °C. This is found to be much more stable numerically. The thawing depth is defined as the -1 °C isotherm. Figure 3.7 compares the results: the analytical solution given in GEO-SLOPE™ (2004), the numerical solution of TEMP/W, where in one case infinite elements are applied in order to realise the boundary conditions. This solution is in better agreement with the analytical solution as the latter one assumes a semi-infinite column.

Another model for comparison considers variations in permafrost thickness in response to changes in palaeoclimate. Osterkamp and Gosink (1991) use a step palaeotemperature model for the surface temperature of permafrost at Prudhoe Bay, Alaska, modified from a model by Brigham and Miller (1973). As far as initial and boundary conditions are stated (see table 3.7), they were implemented in a SHEMAT model. The permafrost depth was calculated following Osterkamp and Gosink (1991) as the -1 °C isotherm. Since some information such as thermal capacity and thermal properties of the rocks could not be reconstructed completely, there is an offset of 200 m between both variations of permafrost thickness. This value was subtracted from the original data of Osterkamp and Gosink (1991), to demonstrate the good (relative) agreement between the two models (figure 3.8). According to Osterkamp and Gosink (1991) the observed current thickness of permafrost at Prudhoe Bay is about 600 m, so that the model underestimates the thickness by 14 % while the (unshifted) model of Osterkamp and Gosink (1991) overestimated by 18 %. The uncertainty in the specific heat flow measurement at Prudhoe Bay is 15 %, thus both results are
3. Palaeotemperature reconstructions for the Kola peninsula and Northern Poland

![Graph showing comparison between SHEMAT and TEMP/W module within GeoSlope™](image)

**Fig. 3.7:** Comparison between SHEMAT and a verification example of the TEMP/W module within GeoSlope™.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid size; Resolution</td>
<td>10 x 900; 1 m</td>
</tr>
<tr>
<td>Basal specific heat flow</td>
<td>0.06 W m⁻²</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.4</td>
</tr>
<tr>
<td>Matrix thermal capacity</td>
<td>2.06 MJ m⁻³ K⁻¹</td>
</tr>
<tr>
<td>Matrix thermal conductivity</td>
<td>3.39 W m⁻¹ K⁻¹</td>
</tr>
<tr>
<td>Total Simulation time</td>
<td>100 ka</td>
</tr>
</tbody>
</table>

**Tab. 3.7:** Parameters of the model adapted from Osterkamp and Gosink (1991).

more or less still within the error range. Figure 3.8 demonstrates impressively the importance of properly accounting for latent heat effects by comparison with a model neglecting those.

### 3.3 Permafrost and the reconstruction of past surface temperatures

The inclusion of the latent heat effects is of outstanding importance when analysing the signal of palaeoclimate. This can be done by inverting for Ground Surface Temperature Histories (GSTH), using an inversion scheme based on nonlinear Tikhonov inversion. Regularisation is achieved by minimising the (semi)norm of a roughening operator applied to the discrete series of temperatures representing GST. The details of this approach are given in section 1.2.2. To deal with permafrost effects, the forward modelling code used in this inversion was replaced with a one-dimensional implementation of the algorithm described in the previous sections of this chapter.

#### 3.3.1 Synthetic example

As a simple example, a boxcar time function is used which is characterised by a temperature decrease of -9 K (from 1 °C) at 65000 years before present, returning to 1 °C at 15000 years before present, marking
the fast warming at the end of the last glaciation. The subsurface was assumed to be uniform with respect to petrophysical properties. Figure 3.9 shows synthetic temperature logs for different porosities, as well as the maximum deviation induced by the inclusion of permafrost effects.
Fig. 3.10: Influence of permafrost formation on ground temperatures for a simple homogeneous model. Left: Temperatures in the top 500 m of the model. Right: Ice content of the porous medium. A value of 1 implies that all porosity is filled up with ice. It is very clear, that a significant temperature signal or even ice relics can be expected in areas of high porosity, even today.

To demonstrate the effect on palaeoclimate inversions, a high porosity of 30 % was chosen for future analogies. As pointed out above, the existence of high porosities are essential for permafrost effects to be significant. The results are shown in figure 3.10. It shows clearly that under favourable conditions, the effects of permafrost from the last glacial should be visible at depth even today. A recent indication of this is given by Safanda et al. (2004) where other independent data are presented supporting the deep occurrence of palaeo-permafrost. Synthetic borehole temperature logs were generated from this simulation, adding normal random noise with a standard deviation of $\sigma = 0.25 \, K$ and a mean of zero. The resulting data set was then inverted, accounting for and ignoring permafrost effects. The difference between including and ignoring the latent heat effect in the inversion algorithm is shown in figure 3.11: the sharp increase due to the step function is much better reproduced when inverting with freezing. It has to be remarked, however, that the porosity assumed is rather high. In practice, effects may be smaller or even negligible in crystalline areas. The boxcar forcing function used for the simulation is a hard case for straightforward smoothing inversions, like the one applied here.

3.3.2 Palaeotemperatures from inversion on the Kola Peninsula

Data from the immediate surroundings of the Russian super-deep borehole on the Kola Peninsula (SG-3) shown in figure 2.9 and described in chapter 2 is used for palaeotemperature reconstructions. Since for most of these boreholes laboratory measurements of thermal conductivities and heat capacities were available at ambient and elevated temperatures, a detailed model of the thermal properties of the subsurface could be set up. For this purpose the measured data were interpolated to the modelling grid, and the temperature dependencies of $\lambda_m$ and $(\rho c)_m$ found from the laboratory measurements were applied to each borehole. The logarithmic modelling grid representing the upper crust extends to 6 km and 8 km with 301 and 501 nodes using data from the shallow holes and the SG–3 hole, respectively. In both cases, the simulation period comprises the last 150 ka discretised into 257 logarithmic steps which accounts for the
coarser resolution at earlier times. The inversion grid, which represents the GST history, is parameterised into 32 logarithmic steps. Although the models for the inversions are one dimensional, the detailed thermal conductivity logs (see figure 2.8) are considered, as well as the variation of thermal conductivity and capacity with temperature (see section 1.2.2). Furthermore, in section 2.4.1 it is shown that the inclined layers of the Pechenga structure only yield a small fraction (less than 5%) of channelling of specific heat flow. The error in measurements of the thermal properties are within the same range so that the effect can be safely neglected.

Shallow boreholes

From individual inversions of single boreholes, those boreholes with the best fits were selected. In particular, temperature logs showing signature of fluid flow or other unexplained features were excluded. First, the possible impact of permafrost development is studied in an inversion of borehole 3359 (see chapter 2). Figure 3.12 shows the result, including and ignoring latent heat effects. As the boreholes are all in crystalline units, a low mean porosity of 1% was assumed. In the light of the parametric studies presented in chapter 5 it can be expected that the effect is negligible, which is confirmed by this result. Therefore, all subsequent results from the Kola peninsula are obtained by purely conductive models, neglecting latent heat effects. For all boreholes, forward simulations were performed prior to the inversions. By varying the basal specific heat flow (at 6000 m depth for the shallow holes and 8000 m for the SG-3) within few mW m$^{-2}$, as well as the present GST within some tens Kelvin, an optimal fit with temperature logs was found. The corresponding values are shown in table 3.8. These values differ from those obtained earlier in section 2.2.3, shown in table 2.2. This emphasises that palaeoclimatic investigations are necessary when determining basal specific heat flow values.

Site 3396 was carefully inverted choosing large trade off parameters $\tau_i$ to obtain a smooth a priori model (see section 1.2.2). This borehole lies some 50 km south of the Pechenga structure in an area with lower
Fig. 3.12: Comparison of GST history reconstructed for borehole 3359 from inversion including (black) and ignoring latent heat effects (grey), together with their standard deviation (broken lines). The difference is barely visible.

<table>
<thead>
<tr>
<th>Borehole</th>
<th>depth (m)</th>
<th>Specific heat flow (mW m⁻²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2271</td>
<td>136 (50–1364)</td>
<td>45.</td>
</tr>
<tr>
<td>2908</td>
<td>1270 (50–800)</td>
<td>45.</td>
</tr>
<tr>
<td>3200</td>
<td>1720 (50–1720)</td>
<td>47.</td>
</tr>
<tr>
<td>3209</td>
<td>806 (50–806)</td>
<td>46.</td>
</tr>
<tr>
<td>3356</td>
<td>1063 (50–1063)</td>
<td>46.</td>
</tr>
<tr>
<td>3359</td>
<td>959 (50–959)</td>
<td>47.</td>
</tr>
<tr>
<td>3396</td>
<td>800 (50–800)</td>
<td>38.</td>
</tr>
<tr>
<td>2915</td>
<td>1270 (50–1270)</td>
<td>47.</td>
</tr>
<tr>
<td>2400</td>
<td>1589 (50–1589)</td>
<td>48.</td>
</tr>
<tr>
<td>SG-3</td>
<td>9000 (500–3500)</td>
<td>48.</td>
</tr>
</tbody>
</table>

Tab. 3.8: Boreholes used in this study (see figure 2.9). Intervals used are given in brackets behind the depth. Specific heat flow was determined prior to the inversions by an optimal fit of forward models with the temperature logs.
3.3. Permafrost and the reconstruction of past surface temperatures

Fig. 3.13: Left: Individual inversions for 8 sites. Also shown is the very smooth prior used in the subsequent inversions (dashed black line). Right: Results from an experiment inverting only N-1 temperature logs from N. Sites 3200 and 3396 dominate the joint curves.

Fig. 3.14: Left: Joint inversions for 7 sites with different priors. Right: Residuals for all logs for the model with the 3396 prior model, which gives the best fit for this choice of regularisation parameters.

relief and is thus believed not to be significantly influenced by deep groundwater flow. The resulting GSTH was used alternatively to zero priors for many subsequent inversions. Figure 3.13 displays all the single site inversions. Joint inversions for all 7 sites are shown in figure 3.14. All results yield relatively moderate Weichselian temperatures, only 4 K – 7 K lower than today. The discussion is given in section 3.3.5.

The importance of accurate thermal properties, in particular thermal diffusivity, is underlined by figure 3.15. An increase or decrease by 20% yields significantly different models for the GSTH. This demonstrates that when inverting borehole data, it is crucial to have sufficient information on thermophysical properties, as well as their variation with temperature (and pressure).
Palaeotemperature reconstructions for the Kola peninsula and Northern Poland

Fig. 3.15: The influence of varying thermal diffusivity on the reconstructed GST histories ($\kappa = 0.9315 \text{ m}^2 \text{s}^{-1}$, dark grey: +20%, light grey: -20%).

Super-deep borehole

To complement the studies presented above with respect to the resolution of Weichselian palaeotemperatures, part of the data from the SG-3 borehole was also inverted. The top 500 m, and the parts below 3500 m had to be neglected due to obvious effects of fluid flow or other problematic features. The data is shown in figure 3.16 together with the typical residual of a single site inversion of SG-3.

The best fit to the borehole data was obtained with a recent mean annual ground surface temperature of 3.5 °C, which is consistent with the studies of Popov et al. (1999b). Since there is a large number of well-determined thermal properties, it is assumed that the basal specific heat flow determined from the temperatures is well constrained to approximately, 48 mW m$^{-2}$ at a depth of 8000 m (see table 3.8), where the effect of heat production is taken into account. This value agrees well with the results from the 3-D model shown in figure 2.18.

The best RMS for this fit is RMS=0.84, with maximum residuals of RMS=1.5 K. The inverted palaeoclimatic is shown in figure 3.17. All inversions including SG-3, whether individual or joint, are much steeper than the ones from shallower boreholes, and display a GSTH with lower Weichselian temperatures near -9 °C. This is significantly lower than the ones estimated from the shallower boreholes. However, the reliability of these results is questionable because they may also be due to (1) the temperature log being not in steady-state conditions; (2) the well known effect of logs of insufficient length (see Hartmann et al. 2005); (3) the smoothing effect of the regularisation employed (see chapter 4), or (4) the uncertain in-situ values of the thermophysical parameters. Moreover, the joint inversion with the shallower boreholes led to much less robust results in the inversion. Although the shallow boreholes are not deep enough to obtain the full signal of the transient surface temperature changes for several tens of thousands of years, it is argued that the initial surface temperature can be determined nevertheless from the curvature of the temperature log. Due to the diffusive character of the temperature signal a steady state condition is assumed at the starting time of the inversion. All temperature before this shows up only in this "pre-observational"
Fig. 3.16: Temperatures ($T$), thermal conductivities ($\lambda$) and one of the best residuals ($\Delta T$) from the SG-3 single site inversion. In this case $\tau_1 = 20$ yielded best results. The corresponding fit was reached for $\text{RMS}\approx 0.8$ and is nearly four times more than for the best fits for the shallow boreholes. Zero priors were used. The arrows mark the part of the temperature log used in the inversion.

mean. In this more flexible code, this initial condition can be used as a prior. However, the time of the postglacial warming as well as any structures in the GST history is not resolved. A prerequisite for this are densely sampled, reliable data. Therefore it is concluded that inversions from the shallow boreholes can produce reliable for Weichselian temperatures as well, which were about 4 K to 7 K lower than today. This is in agreement with the general result by Kukkonen and Jöelehtä (2003) (see section 2.4.2) who obtain a postglacial warming of $8 \pm 4.5$ K. Thus, the temperature step to the Pleistocene is smaller than observed in lower latitudes (see section 2.4.2). Nevertheless, to study the maximum influence of the palaeoclimatic disturbance, the forward simulations in section 2.4.2 consider also a larger steps of 9 K and 15 K.

Fig. 3.17: Estimated GSTH from the SG-3 deep borehole. Also shown is a typical result from the joint inversion of the shallower boreholes. Zero priors were used for both results.
3.3.3 Palaeotemperatures from inversion in northern Poland

The inversion procedure is also used to interpret temperature data from a borehole, UDRYN IG-8, located in the sedimentary basin northeastern Poland. In this borehole, not only temperature data was available, but also porosities and thermal conductivities reconstructed from borehole wireline logging. Due to some disturbances in the uppermost part of the temperature log, only data from below 100 m depth is used. A simple layered model is applied, compiled by Majorowicz. The data for this borehole is shown in figure 3.18. It shows that porosity is sufficiently large to warrant a significant impact of the thawing or freezing process. For the inversion, the extent of the forward model had to be set to a depth of 5000 m, assuming the properties below the depth of the borehole to be mean bedrock properties as found in the borehole below 900 m. Formulations for the temperature dependence of the thermal properties were adopted from Haenel et al. (1988) for thermal conductivity, and from Herrmann (1999) for heat capacity. Water properties were calculated as a function of temperature and pressure (see section 3.1.2). Ice properties and the freezing function are the same as in the forward code presented above. Boundary conditions were set as follows: At the top, a variable ground surface temperature history is assumed. The best fit to the borehole data was obtained with a recent mean annual temperature of 7 °C, which is slightly above the mean annual air temperature of 6 °C (2 m above ground) at the location of the borehole. As thermal conductivity is assumed to be basically correct, there is not much freedom to vary the basal specific heat flow, which is 38.4 mW m⁻² at a depth of 5000 m, when accounting for the effect of radiogenic heat production. This corresponds to a surface specific heat flow of 41.4 mW m⁻² which has been determined by Majorowicz. Temperature data was smoothed and interpolated to the modelling grid. A logarithmically scaled time step is used, starting with large time steps in the past from 150 ky to small steps up to the present.

From experiments with the inversions of truncated logs it is found that RMS = \( \sqrt{\frac{1}{N} \sum (T_{obs} - T_{calc})^2} \) of the best fit which could be obtained increased systematically with the depth of the logs (see figure 3.19).

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1 personal communication by J. Majorowicz, Northern Geothermal, Edmonton, Canada
This suggests that some depth dependent petrophysical parameter variations have not been sufficiently accounted for. For instance, a general relationship from crustal-scale studies is used for the temperature dependence of thermal conductivity and capacity. It may be necessary to adapt the coefficients of these polynomial representations to the sedimentary environment at the UDRYN site. Also, heterogeneities at larger depths should be taken into consideration. For this reason, only the data above 1500 m of the depth of the borehole are used in the inversion. The GSTH is parameterised by a piecewise constant function, with a logarithmically decreasing time interval. For the particular inversions shown, the number of degrees of freedom is limited to 64. A logarithmic time step size is well adapted to the fact that the temporal resolution of borehole data decreases with time. The inversion is run with different smoothness constraints which determine the balance between roughness and data fit (see chapter 4). For the results shown below, the regularisation parameters are set to the values corresponding to lowest values which yield a stable result. As using a constant prior implies an unrealistic assumption of mean temperatures before the initiation of the simulation, a smooth transition is chosen from the recent GST of 7 °C to an initial value of -9 °C. This particular prior model entering the regularisation was inspired by the results of Šafanda et al. (2004). The results from the inversions are given in figure 3.20. Although these inversions may be improved following the suggestions given above, several conclusions can be already drawn: Given a fixed regularisation, the inclusion of latent heat effects improves the data fit significantly. Additionally, the resulting GSTH appears to be more consistent with the generally accepted timing the end of the Weichselian glaciation some 14 ka to 15 ka ago (Hartmann, 1994). The lowest temperature resulting from the inversion is about -11 °C. From these results, the history of subsurface temperatures and the amount of ice content is calculated.

In general, these findings agree well with those of Šafanda et al. (2004), who present forward modelling...
**Fig. 3.20:** Comparison of the results from the palaeoclimatic inversions for GST from the UDRYN borehole. The black curve represents the results including latent heat effects, while the grey line is the result obtained from standard assumptions. The former fits the data better which is indicated by a much lower RMS. The large difference is mainly due to the very high porosity in the upper 900 m (see figure 3.18). Both curves refer to baseline of $7^\circ$ C, i.e. the zero level corresponds to this value. The inset shows the prior model entering the inversion.

**Fig. 3.21:** Permafrost formation at the UDRYN site from the inversion model shown in figure 3.20. Left: Temperatures ($^\circ$ C) in the top 800 m of the model. Right: Ice content in the porous medium. A value of 1 implies that all porosity is filled up with ice. Defining permafrost thickness by the $-1^\circ$ C isotherm (white line), it reaches a maximum depth of 650 m shortly after the beginning of the simulation. No ice is present after $\approx 4$ ka B. P. The ice content is scaled as in figure 3.10. In contrast to this homogenous model, the actual amount of ice and latent heat here depends on the variable porosity.
results including permafrost for the same borehole. The minimum temperature obtained by the inverse model (-11 °C) is nearly the same as the one given by these authors. As in their model, permafrost disappears at about 4 ka B. P. (see figure 3.21). The maximum permafrost depth defined by the -1 °C isotherm, however, is larger in this model (≈ 650 m in contrast to ≈ 520 m). This is probably due to differences in the assumed temperature dependencies in the thermophysical rock and fluid properties. Additionally, the partition function in equation (3.2) is different from the one used by Safanda et al. (2004).
3.3.4 Results from Monte Carlo Inversion

The inversion method used for the determination of GST histories in the previous sections requires, particular a priori models to be specified. In contrast, the Monte Carlo method does not have this constraint. Therefore, this random scheme is useful for testing the results from the systematic inversion. This is carried out for the Polish study area.

As pointed out in section 1.2.2, the use of FD methods within the Monte Carlo inversion requires a moderate number of inversion parameters in order to keep CPU times at reasonable levels. Hence, the temperature history was divided into N=10 steps. The basal specific heat flow is included in the inversion, whereas the present ground surface temperature is kept at the same level of 7 °C as in the systematic inversions. After evaluating 10 000 random models with the Metropolis algorithm, the last accepted model is included in the a posteriori distribution.

This stochastic inversion confirms the importance of including latent heat effects into the modelling. Figure 3.22b shows the result when these effects are accounted for. It is more "stable" with respect to both temperature history and basal specific heat flow as seen by the broadening of the distribution of a posteriori models. The histogram of the latter one peaks at about 44 mW m⁻², which is slightly above the value assumed in section 3.3.3. In general, a comparison of the results in 3.3.3 with this stochastic scanning of the model space yields good agreement, except for very short times (less than 50 a B. P.) and the longest periods (greater than 50 ka B. P.). Considering that the inversion was started at a depth of 100 m, the start period deviation is easily explained. For long periods, the data probably does not carry much information due to the limited length of the temperature log. The smooth behaviour in the Tikhonov inversion for both cases is due to additional prior information included in the deterministic approach.
Fig. 3.22: A posteriori models for the temperature history from Monte Carlo inversions for the UDRYN site. a) Without latent heat effects, b) with latent heat effects. The blue lines show all models, whereas the red lines depict the mean models together with the standard deviation. The insets show the corresponding relative frequencies of a posteriori basal specific heat flow values.
3.3.5 The role of Weichselian glaciation: comparison between the Kola and Poland study area

The palaeotemperature inversions for the Kola area differ significantly from those for northern Poland. Whereas in the former area Weichselian temperatures are only around 7 K lower than today (see section 3.3.2), the data from Poland imply a temperature difference of around 20 K. To explain this behaviour it may be hypothesised that the longer duration of ice coverage in the Kola area during the retreat of the Weichselian glaciation maintained the ground temperature at moderate levels. This implies that temperatures at the base of the ice cover have been only a few degrees below zero. As shown in figure 3.23 at the Polish site, the time of longer exposure of the surface to cold air temperatures during the retreat of the ice may be as much as some thousand years. To test this hypothesis, different forward models of GST histories were run for the model at the UDRYN site. Figure 3.24 shows the results together with the best fit corresponding to the inversion plotted in figure 3.20.

Model M1 (figure 3.24a) represents a longer persistence of cold climate conditions (135 ka), whereas M2 is the model for a longer ice cover, with only a short time period of low temperatures (10 ka). Both models include the end of the glaciation at near 10 ka before present. As seen from figure 3.24b, M1 fits the data asymptotically for deeper parts (corresponding to earlier times), whereas M2 shows a good fit only for the upper part. It is concluded that very low temperatures must have prevailed such as in Model M1 and shown by the inversion, in spite of a possible insulating effect of the ice cover at UDRYN. Either, there were freezing conditions at the bottom of the glacier at UDRYN, or during most of the time period from around 100 ka to 14 ka b. p. the area was not covered by glaciers at all. Figure 3.24 shows also that reducing temperatures before the last glacial maximum at about 14 ka b. p. yields a much better fit (M3). This model considers several temperature steps and the comparison with the other models shows that a simple boxcar model will not explain the data.
Fig. 3.23: Study areas Kola and UDRYN. Isolines show the age (in ka b. p.) of the maximum extent of the glaciation. Redrawn from Kukkonen et al. (1998).

Fig. 3.24: Different step functions (a) used as forcing functions for calculating temperature profiles at the UDRYN site (b) in forward calculations.
3. Palaeotemperature reconstructions for the Kola peninsula and Northern Poland
In the previous chapter it is shown by some synthetic and field examples that the latent heat effects associated with permafrost development in glacial and periglacial areas considerably influence the diffusion of transient temperature signatures into the subsurface. Therefore, inversion methodologies for reconstructing these signals need to account for freezing and thawing processes. This finding motivated a more general and systematic study of the magnitude of these processes, considering how this maybe applied in retrospect to other data sets where latent heat effects are important, but had been neglected in the inversions. However, since such a study requires the solution of many synthetic inverse models, a modification of the code is necessary. As described in section 1.2.2, a regularisation parameter must be chosen in order to find an optimum trade-off between the size of a regularised solution and its fit to given data. So far, this optimal value was found by try and error, but here, an automated determination is required due to the large required number of models runs. This chapter (published in Rath and Mottaghy (2007)) presents this implementation in the inverse code, estimating the best value of the regularisation parameter by the generalised cross-validation method. Field data from the Kola area (chapter 2) and UDRYN borehole (chapter 3) is used to demonstrate the method. The parameter study mentioned above is introduced in the next chapter.

4.1 Regularising operators

Resuming the description of the inverse method from section 1.2.2, the following combination of differential smoothing operators of different order (adapted from 1.23) are used: $L_0 = I$, and $L_1$. This operator represents the discrete first derivative with respect to time, and is defined as

$$L_1 = \Delta t^{-1} \begin{bmatrix} -1 & 1 \\ -1 & 1 \\ \vdots & 1 \\ \beta & -1 & 1 \end{bmatrix}.$$  \hspace{1cm} (4.1)

The product of the matrix defined in equation (4.1) with the parameter vector $p$ may be interpreted as the discrete approximation of its first derivative, where $\Delta t$ is the temporal inverse mesh spacing, which is assumed to be constant for the moment.

If $L_0$ is used, the minimum distance between the solution and the prior model is sought. Regularising with the $L_1$ operator penalises solution roughness, and guarantees smooth solutions if the weighting parameter $\tau$ is chosen large enough. The $L_1$ operator as defined above favours "flat" solutions.
et al. [2002] gives an example of an inversion of a synthetic model with the technique described here and the method of Clauser and Mareschal [1995], Beltrami et al. [1997], and Beltrami and Mareschal [1995]. The current technique makes it particularly easy to include the pre-observational mean temperature (commonly called POM) as a prior, as well as explicit values for basal specific heat flow and current surface temperature. In contrast, the former method determines these parameters from the data. This may lead to the difficulties described by Hartmann et al. [2005], when inverting for GSTH for times further back in the past than about 1000 years. This is clearly visible in figure 4.1, where the minimum at 20000 y. b. p. disappears, when short temperature logs are inverted which are too short. From the penalising of roughness it also follows that longer period noise is still visible in the GSTH.

For the subsequent inversion inversions, the ratio of the two regularisers ($L_0$ and $L_1$) is fixed, simplifying the search for an optimum regularisation. The goal is to find the best value of $\tau$, where $\tau_0 = \tau \tilde{\tau}_0$ and $\tau_1 = \tau \tilde{\tau}_1$ with the tilde denoting the fixed initial values. In principle, however, also a two-parameter search could be employed.

4.2 Choosing the optimum regularisation parameter

Following Farquharson and Oldenburg [2004], the generalised cross-validation (GCV) method is briefly described here. Defining the appropriate value of the regularisation parameter for the GCV criterion is based on the “leave-out-one” lemma (Wahba [1990]). There, the linear inverse problem considered which minimises

$$\sum_{i=1}^{N} [d_i - g_i(p)]^2 + \tau \|p\|_2^2,$$

(4.2)

with respect to the model $p$, where $g(p) = Ap$ is the forward model described by the matrix $A$. The noise in every observation $d_i$ is assumed to have the same standard deviation $\sigma_i = \sigma_0$. If all but the $k$th observation are inverted, setting the regularisation parameter to a trial value $\hat{\tau}$, the problem is now to find the model $p^k$ which minimises

$$\sum_{i=1, i\neq k}^{N} [d_i - g_i(p)]^2 + \hat{\tau} \|p\|_2^2.$$  

(4.3)

If $\hat{\tau}$ is a suitable value for the regularisation parameter, the $k$th forward-modelled datum $g_k[p_k]$ is expected to be close to the omitted observation, $d_k$. Obviously, this procedure can be repeated for each observation $i$. If all the calculated data $g_k[p_k]$ are close to their observations $d_i$, $\hat{\tau}$ can be considered an appropriate value of the regularisation parameter, in terms of the whole minimisation problem. It follows that this value can be found by minimising the function

$$V(\hat{\tau}) = \sum_{k=1}^{N} [d_k - g_k[p_k]]^2,$$

(4.4)

which is called the ordinary cross-validation function. Wahba [1990], pp. 52-55, derives an expression is derived which allows to determine $V_0$ without solving the inverse problem explicitly for each omitted observation:

$$V(\tau) = \sum_{i=1}^{N} \frac{[d_i - g_i(p^\tau)]^2}{[1 - B_{ii}(\tau)]^2}.$$  

(4.5)
4.2. Choosing the optimum regularisation parameter

Fig. 4.1: Result of smoothing Tikhonov inversion (from Clauser et al., 2003). A synthetic temperature log including a palaeoclimate was generated. For this experiment, this log was gradually shortened. Normally distributed noise with mean 0 and a standard deviation of $\sigma = 0.25$ K (i.e., $N(0, 0.25)$) was generated independently for each log, and added to the data. Subsequently, the inversion was done with the Tikhonov algorithm described here (top), and the TSVD technique developed by Beltrami et al. (1997) (bottom). For the smoothing inversion a first order operator was used (equation 4.1). The length of the synthetic log is plotted along the horizontal axis. A comparison of the results shows clearly the robustness of the Tikhonov approach with respect to noise: the resulting GSTHs are much smoother. Moreover, phase and amplitude of the true signal can be reconstructed sufficiently with much shorter temperature logs. Minimum required length is marked by dotted lines.
Here, \( p^\tau = (A^T A + \tau I)^{-1} A^T d \) is the solution of the inverse problem for the particular value of \( \tau \), and \( B_{ii} \) is the \( i \)th diagonal element of matrix \( B(\tau) = A(A^T A + \tau I)^{-1} A^T \).

The general cross validation (GCV) function is invariant under an orthogonal transformation (Wahba 1990):

\[
V_0(\tau) = \frac{\| d - g(p_\tau) \|^2_2}{\text{trace}(I - B(\tau))},
\]

(4.6)

The problem of inverting borehole temperatures for ground surface temperature histories is non-linear, and hence requires the use of an iterative procedure. It was shown in Haber and Oldenburg (2000) that the GCV criterion yields a good estimate of the regularisation parameter, if the non-linear inverse problem is convergent. Using the notations from section 1.2.2 (equations 1.18 and 1.22), the forward model \( A \) is approximated by \( A = W_d J^{n-1} \) at the \( n \)th iteration and the corresponding GCV function is

\[
V_n^0(\tau) = \frac{\| d - g(p_n) \|^2_2}{\text{trace}(I - W_d J^{n-1} M^{-1} J^{n-1T} W_d^T)},
\]

(4.7)

where

\[
M = J^{n-1T} W_d^T W_d J^{n-1} + \tau W_p W_p^T,
\]

(4.8)

and \( \tau_{GCV} \) is found by minimising equation (4.7). In the inverse problem discussed in this work, an initial interval for this parameter is chosen which is gradually narrowed during the following iterations. This reduces the number of necessary calculations of the GCV function. The effort can be further reduced by combining this method with a cooling-type procedure, where a initial (sufficiently large) value of \( \tau \) is constantly reduced for each new iteration before the GCV method is performed.

For demonstrating the power of the proposed method, a slightly smoothed boxcar forcing function is used for calculating a synthetic borehole log and gaussian noise (\( N(0, 0.25) \)) is added. In figure 4.2a, the temperature profile is plotted, together with the GSTH. The upper right panel shows the a posteriori GSTH, where the iteration process is mapped by different colours. The model for each iteration is obtained with an optimised regularisation parameter \( \tau \), found by the minimum of the GCV function \( V_0 \) (equation 4.7) which is plotted in figure 4.2c versus \( \tau \). Here, the iteration number is indicated by the colour-code. Figure 4.2d demonstrates the influence of the regularisation parameters on the reconstructed GSTH in the last iteration: the red line is the model determined by using the regularisation parameter found at the minimum of the GCV function \( V_0 \). Results for the other models are plotted in different grey scales, the darker the closer to the minimum. The resulting GSTH reproduces quite well the true boxcar model, though there are still some artifacts like the maximum near 3 ka. This is believed to be due to the known fact that using GCV estimates for the regularisation parameter can cause to much structure in the model (Walker 1999). In this case a combination of the GCV criterion with a cooling-schedule-type behaviour would be a simple remedy (Farquharson and Oldenburg 2004): The optimum value \( \tau_{opt,n} \) at the \( n \)th is then

\[
\tau_{opt,n} = \max(a \tau^{n-1}, \tau_{GCV}),
\]

with \( a \) being an appropriate number between 0.01 and 0.5.

Though the GCV method was used in a straightforward manner in this study, it must be mentioned that optimum values of the regularisation parameters can also be found by more advanced techniques, if computer resources become important due to the size of the problem (see Golub and von Matt 1996). An alternative method to speed up the solution of equation 1.22 for multiple \( \tau \) is a modification of CGLS
4.2. Choosing the optimum regularisation parameter

Fig. 4.2: Results from GSTH reconstruction from a synthetic example with an optimised regularisation parameter. (a) Synthetic temperature log resulting from the forcing function in the inset. (b) Reconstructed GSTH for each iteration, where the colours correspond to the iteration number. (c) GCV functions for each iteration (same colour code as in b). (d) Reconstructed GSTH for the last iteration (red). Also shown are results for different values of the regularisation parameters at this iteration, where the grey scale indicates the distance to the minimum.

4.3 Example 1: Kola Peninsula, Russia

In this example, the same data as in section 3.3.2 is analysed, using the available temperature log from the Kola super-deep borehole SG-3. The GCV procedure described in section 4.2 is applied to this data set, using a zero prior model. In this case the GCV functions are rather smooth in the later iterations, indicating that the final model is robust with respect to the choice of \( \tau \) (figure 4.3c). Comparing the results (figure 4.3) with those from section 3.3.2, it can be seen that the modified inversion method yields temperature histories which are more consistent with those obtained from the shallow boreholes of the Kola area (figure 3.13): The Weichselian temperatures are only 6 K -7 K lower than today, similar to the results from the shallow holes. Earlier results for the SG-3 suggest a larger temperature step (\( \approx 9 \) K). Thus, it is obvious that the regularisation method may have a significant impact on the inversion result. Obviously it yields a more objective result, because in section 3.3.2 it was concluded differences between inversions may be due to the regularisation method applied in each case.

The best fit to the borehole data was obtained with a recent mean annual ground surface temperature of 3.5 °C, which is consistent with the findings of Popov et al. (1999b). Due to the large number of well-determined thermal properties it can be assumed that the basal specific heat flow determined from the temperatures is well constrained at approximately 48 mW m\(^{-2}\) at a depth of 8000 m where the effect of heat production is taken into account.

4.4 Example 2: Udryn, Northeastern Poland

A second field example uses data from the UDRYN IG-8 borehole which were already presented in Šafanda et al. (2004) and chapter 3 (figure 4.4a). As pointed out in section 3.3, the information on porosity is important in this case as, in contrast to the previously discussed SG-3, porosities are large enough to warrant a significant impact of thawing or freezing. For the inversion, the depth of the forward model had to be limited to 5000 m, assuming the properties below the depth of the borehole to be mean bedrock properties as found in the borehole below 900 m. For the temperature dependence of the thermal properties of the rocks, the same approach is used as described in section 3.3.3 was applied. Water and ice properties were calculated as a function temperature and pressure (see section 3.1.2). Boundary conditions such as mean annual surface temperature and basal heat flow as well as inversion grid properties are the same as in section 3.3.3.

For the inversion, a zero prior is used again. Figure 4.4 shows that the GCV function stabilises only after quite some iterations. In this case, combining the GCV method with a cooling-type procedure might help, where a starting large value of \( \tau \) is constantly reduced during the first iterations before the GCV method is applied.

4.5 Discussion

The specific method applied in this study raises several questions. Using this technique, the aim is to reduce significantly the interpreter’s role in GSTH inversions. Though an appropriate method for the
Fig. 4.3: Results from GSTH reconstruction for the Kola super-deep borehole with an optimised regularisation parameter. Panel (a) shows temperature $T$ and thermal conductivity $\lambda$ versus depth. The arrows mark the interval used for the GSTH inversion. For meaning of the other panels see figure 4.2.
Fig. 4.4: Application of the GCV technique to the UDRYN borehole (Northeastern Poland). Panel (a) shows the temperature log (T), porosity (φ), and the thermal conductivity (λ) distribution. For meaning of the other panels see figure 4.3.
4.5. Discussion

The selection of the regularisation parameters was successfully set up, several questions are still open.

First of all, one may argue that the rather fine temporal discretisation used may be an over-parametrisation. It is indeed, given the resolution of borehole temperatures. However, it is one possibility for combining flexibility with respect to the unknown time history of GST with the incorporation of prior knowledge. Due to the fine resolution of the step function used for driving the model, the assumptions about the palaeotemperature history are kept to a minimum. Furthermore a logarithmically equidistant setup of steps leads to a well-adapted inverse mesh, placing more parameters where resolution is possibly high, and less where only long-period signals have survived.

The necessity for regularisation is obvious in a severely ill-posed problem like GSTH inversion. The approach taken in this study uses a combination of Tikhonov regularisation operators, which at first glance may be thought to be arbitrary. However, the particular choice here for the regularisation matrix can be understood in an informal way from a Bayesian point of view. There is a close connection of difference operators to the inverse covariances used in this approach. It has been pointed out several times (Xu, 2005; Tarantola, 2004; Yanovskaya and Ditmar, 1990; Tarantola, 1987) that the inverses of exponential or gaussian covariances may both be approximated by a weighted sum of a diagonal and the squared $L_1$ matrix. In particular, an expression for the Markovian (exponential) covariance

\[ C_{ij}^M = \sigma^2 \exp \left( -\frac{|i-j| \Delta t}{\xi} \right) \]

in terms of the differential operators was given by Rodgers (2000). Here $\xi$ is the corresponding correlation time. With $\gamma = \exp(-\Delta t/\xi)$ it is

\[ (C^M)^{-1} \approx \frac{\alpha}{\sigma^2} \left( \frac{1}{\alpha} I + L^T L \right), \tag{4.9} \]

where $\alpha = \frac{\gamma}{1 - \gamma^2}$. Interpreting the determination of the optimum $\tau$ as a crude empirical estimation of hyper-parameters (Mitsuhata, 2004), one can see that $\tau_{opt} = \sqrt{\frac{\pi}{\alpha}}$, and $c = \alpha^{-1}$, from which estimates of $\sigma$ and $\xi$ could be calculated. In this study, the relative weights of $L_0$ and $L_1$ are fixed for a given problem with a single tuning parameter, $\tau$, remaining. In principle, also a simple two-parameter search could be employed. In this scheme, usually a logarithmic inversion grid is employed. This turns out to be an effective means to take into account the decreasing resolution of borehole temperatures with depth, though it much simpler than the approach of Serban and Jacobsen (2001).

The results from the case studies presented above are encouraging. Not only did the GCV method converge, but also led to meaningful results in every case given. In all cases, zero priors were used, explaining the behaviour of the curves obtained. Note that the roughness penalty is applied to the deviation from this prior, not to the model. Both field data sets were cleaned for near-surface spurious effects. As already mentioned above, Kola SG-3 was used from 500 m to 3500 m, leaving the last millennium badly constrained by the data, but strongly influenced by the prior and regularisation. At the UDRYN site, the situation is similar, with the top of the data used at 150 m. This implies, that the apparent medieval climatic optimum in both of these results may be an artefact of the smoothing technique and the missing data for the top few hundreds of metres.

GST changes before 20,000 a B. P. will probably not be resolved by the data. This is due both to the uncertainties in the model such as the specific heat flow estimate used, and the data.
4. Objective and automatic inversion for GST histories
5. PROPOSAL FOR A CORRECTION OF EXISTING GST HISTORY INVERSIONS FOR LATENT HEAT EFFECTS

In this chapter, a more general and systematic study of the influence of the latent heat effect in GST history inversions is presented. A selection of several different climate scenarios, kept as general as possible, allows to give a quantitative statement on the different results when latent heat effects are either included or omitted in the inversion calculations. This comprehensive study in turn had motivated the modification of the inverse code which was presented in the previous chapter. The results may be applied to existing inversions which were obtained in boreholes where temperatures are or used to be low enough and where the bedrock has a significant porosity. This applies to areas in North America, such as the Great Plains, where quite a few borehole data exists. However, these are mostly only a few hundred metres deep which is too shallow for detecting the signal of the last ice age. Borehole data from Europe and Asia seem to be more appropriate. As shown in chapter 3, in particular deep boreholes on the East European Platform come into consideration, as well as boreholes in Central Europe and in Russia.

5.1 Synthetic models

The quantitative determination of the influence of latent heat effects on GSTH inversions on the one hand requires considering a wide range of parameters and temperature histories, on the other hand it is necessary and inevitable to keep the scenarios sufficiently general and computing times reasonably short.

To achieve this, a simple step function at 15 ka B. P. is used as forcing, going from a past low temperature level to today’s higher temperature. Total simulation time is 150 ka. The size of the temperature step \( \Delta T \), representing the warming from Pleistocene to Holocene varies between 10 K and 20 K. The timing of the step at 15 ka B. P. is believed to be a characteristic for moderate and high latitudes. Today’s ground surface temperature is varied between 2 °C and 12 °C, to allow for different recent climate conditions. These values and the climate histories which are used in the subsequent models are summarised in table 5.1. The combination of all possible models with these parameters yield a total of 432 synthetic homogenous mod-

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<tr>
<th>Climate History</th>
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<tr>
<td>( \Delta T ) (K)</td>
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<td>Time of temperature step (ka B. P.)</td>
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<th>Subsurface properties</th>
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<td>Thermal conductivity ( \lambda ) (W m(^{-1}) K(^{-1}))</td>
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<td>Thermal capacity ( c ) (MJ m(^{-3}))</td>
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<tr>
<td>Porosity ( \phi )</td>
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</tbody>
</table>

*Tab. 5.1: Parameters of the different synthetic forward models. All possible combinations yield a total of 432 models.*
els, each to be used in two inversions accounting for and neglecting latent heat effects. This large number of model runs requires an automatic determination of the regularisation parameter $\tau$. Determination by trial and error would not be possible within acceptable time. Nevertheless, the total computing time on a 1.8 GHz Opteron workstation summed up to 10 days for all models. As an example, figure 5.1 illustrates one result of a particular combination of parameters.

5.2 Results and discussion

The interpretation of subsurface temperature changes due to GST variations since the last glaciation is focused on the difference $\Delta T$ between today’s mean GST and the one prevailing during the last glaciation. In particular, it is studied how the estimated $\Delta T$ varies in response to the variations in the parameters shown in table 5.1.

As demonstrated for the UDRYN borehole (see figure 3.20), neglecting latent heat effects results in an overestimation of $\Delta T$. The aim is to quantify this difference $T_{\text{diff}}$ (see figure 5.1) in order to correct existing, previous inversions from locations where permafrost may be relevant. When using field data, the a priori surface temperatures and thus $\Delta T$ are not known but need to be determined by the inversion itself. Therefore, temperature differences $T_{\text{diff}}$ are determined with respect to a total of six temperature steps $\Delta T$ from 10 K – 20 K for all 72 parameter combinations (see table above). From this, the arithmetic mean $T_{\text{diff}}$ and standard deviation $\sigma$ of these values are determined.

The result is shown for $\phi = 0.1$ (figure 5.2), $\phi = 0.2$ (figure 5.3), and $\phi = 0.3$ (figure 5.4). Panels (a) show $T_{\text{diff}}$, panels (b) shows the corresponding standard deviation $\sigma$, both plotted versus specific heat flow and today’s surface temperature $T_0$. Clearly, porosity is the most important parameter: In the case of $\phi = 0.1$, $T_{\text{diff}}$ is close to $\sigma$, thus only a trend can be observed, which becomes clearer in figure 5.3. Generally, the effect is largest at low present day GST and low specific heat flow values. The largest values of up to 4 K result for $\phi = 0.3$ (figure 5.4), again for low GST, but at moderate specific heat flow values around 40 mW m$^{-2}$ to 60 mW m$^{-2}$. This shows that not only a large porosity and low mean surface temperatures are required for a large effect but that also the absolute temperature in the subsurface is important which is related to the basal specific heat flow. A larger temperature gradient which occurs for the same GST history at higher specific heat flow values causes a longer persistence of the temperature field within the freezing range. This in turn results in larger amount of latent heat being consumed or released.
Fig. 5.1: An example from the set of model runs. (a) including and (b) neglecting latent heat effects. Porosity is 0.2. The inset in (b) shows the forcing function applied to the forward models. The inversions in (a) and (b) yield different temperature steps $\Delta T_{\text{inc}}$ and $\Delta T_{\text{neg}}$, which define a difference $T_{\text{diff}} = \Delta T_{\text{neg}} - \Delta T_{\text{inc}}$. The iteration number is indicated by the color code.
5. Proposal for a correction scheme of existing GSTH inversions

**Fig. 5.2:** (a) Temperature difference $T_{diff}$ between inversions with and without latent heat effects at $\phi = 0.1$. (b) $\sigma(T_{diff})$, both plotted versus basal specific heat flow and today’s temperature assumed in the forward models.

**Fig. 5.3:** Temperature difference $T_{diff}$ and $\sigma(T_{diff})$ as in figure 5.2 for $\phi = 0.2$. 

**Fig. 5.4:** Temperature difference $T_{diff}$ and $\sigma(T_{diff})$ as in figure 5.2 for $\phi = 0.3$. 

\[ \text{Today’s ground surface temperature } T (\degree C) \]

\[ \text{Basal Heat Flow } q (\text{W m}^{-2}) \]
6. CONCLUSIONS AND OUTLOOK

Numerical modelling based on thermophysical data is a powerful tool and crucial for studying and identifying heat transfer processes in the upper crust. This is demonstrated in a case study for the Kola area where a considerable amount of data is available. It is shown that a combination of forward and inverse modelling has a high potential for quantifying and identifying different heat transport processes. In particular, flexible forward and inversion codes allow to account for the different temperature dependencies of the thermophysical properties of the local rocks. This turned out to be important for both simulation modes: In order to explain the measured data by forward modelling, as well as for the success of the inversion, the variation of the properties must not be neglected, since it can affect strongly the estimation of Weichselian palaeotemperatures. Therefore, the comprehensive data set on thermal rock properties from the Kola region form an excellent basis for geothermal modelling. The analysis of temperature dependence of the important parameter thermal diffusivity shows a significant variation, since both specific heat capacity and thermal conductivity contribute to it. These results have motivated an ongoing study (Mottaghy et al., 2007) in which the temperature dependence of thermal diffusivity between rocks from the Transalp project (Vosteen and Schellschmidt, 2003) and this study are compared.

In spite of these numerous thermophysical measurements, other parameters must enter the numerical models. Very important is permeability, but data is generally sparse for the crystalline environment of the Kola area. Additionally, no geophysical logs were available from the several shallow boreholes, so that a regional model had to be set up using general geological information. Being aware of these constraints, the three-dimensional modelling showed that in the Kola area advective heat transport dominates the vertical specific heat flow distribution if the available data on permeability is invoked. However, sensitivity studies show that these values are in a sensitive range, meaning that a little increase or decrease may have a large effect on the results.

Transient simulations indicate that changes of ground surface temperatures cannot be neglected, since they may also cause a significant variation in specific heat flow. In areas with less relief energy and correspondingly less heat advection this can become the predominant effect. However, in order to explain the data, especially those from the deeper part of the super-deep borehole, some uncertainties remain, particularly with respect to the pressure dependence of thermal conductivity and thermal capacity.

In the present study by Mottaghy and Rath (2007), a local, larger scaled three dimensional model will be discussed. In spite of the lack of accurate permeability and elevation data at a larger scale, it is hoped to further quantify the physical reasons for the specific heat flow variation, in particular the GST history. Other local circumstances like the deep open pit mines near some shallower holes must be included in the considerations. This work will be followed by another study, regarding three dimensional inverse modelling. This will allow optimal parameter estimation and an uncertainty analysis.

The inverse code applied here allows to reconstruct the thermal signal of past climate from deep borehole temperatures for the last few ten thousand years. This implies that many areas which no longer show signs
of permafrost have been exposed to low temperatures and possibly permafrost during this period. Therefore, the inclusion of the thermal effects of permafrost is essential when aiming at the reconstruction of consistent spatial distributions of past temperatures over large regions. Hence the influence of permafrost has been implemented both in the forward and inverse code. After a successful verification by comparing the model with analytic solutions and independent numerical simulations, this new approach is tested on field data. The results confirm that freezing and thawing effects significantly alter the inversion results. This implies that wherever high porosities exist, latent heat effects must be considered. Regional and local fluid flow is also important in permafrost regimes. Therefore, in order to study these regimes, flow must be included into the simulations. Only in this way the effects of the coupled forcing of climate and fluid flow can be studied. This study showed that this is a requirement for a consistent reconstruction of palaeotemperatures, in particular in areas where significant advection can be expected.

GSTH inversions from the Kola Peninsula and northern Poland yielded the unexpected results that GST during the last glacial maximum are considerably lower at moderate latitudes. For the Kola area, temperatures turned out to be 4 K to 7 K lower than today with a good fit (RMS ≈ 0.3 or better), whereas temperatures in northern Poland were some 18 K lower than today (RMS ≈ 0.9).

Independent sources suggest that the Kola area was covered by ice much longer than Northern Poland (e.g. Siegert and Dowdeswell 1998). Near-melting conditions at the base of the glacier at Kola could explain the warmer palaeotemperatures in the inversions for this area. However, the very low temperatures are not consistent with the assumptions of temperate conditions at the base of the Weichselian ice sheet in northern Poland. While the difference in retreat history of this ice sheet cannot explain the data completely, a long time of exposure to cold climate conditions before the last glacial maximum may be a possible explanation. Combining glacier models with subsurface heat transport models may help to reconcile competing assumptions. Besides these considerations, the implication for moderate Weichselian temperatures in the Kola area is in agreement with the general result by Kukkonen and Jõeleht (2003) who obtain a postglacial warming of 8 ± 4.5 K from an analysis of numerous vertical specific heat flow profiles on the Fennoscandian Shield and the Eastern European Platform.

In the crystalline environment of the Kola peninsula with negligible porosity, the latent heat effect need not be considered. In contrast, the results for northern Poland emphasises the importance of accounting for freezing and thawing processes. Therefore, a parametric study is presented, which allows to quantify to a certain extent the deviation between inversion results with or without latent heat effects regarding other factors like specific heat flow, ground surface temperature, and the magnitude of the post glacial warming besides the important parameter porosity. In spite of the simplifications made when setting up the synthetic models, the results may be applied to correct previous inversion results, where the latent heat effect had been neglected. Future work will address to a similar approach regarding the inversion of short term ground surface temperature histories, going back only some hundred years.

This parametric study required the development of a method for selecting the optimum regularisation parameter for smooth palaeoclimatic inversions. This is essential for keeping the computing times of the inversions at an acceptable level. But this promising technique also makes the GSTH inversions more automatic and more objective. Manual intervention of the interpreter is reduced in the sense that once the regularising operator (L_1 in equation 4.1) is selected, the trade-off parameter is chosen in a reproducible manner. The power of this approach, called the general cross validation (GCV), is demonstrated both on synthetic data and on two field examples. Although the convergence histories display quite different
features in the three cases, a satisfactory final result was obtained in each of them. Thus, the method
implemented here shows robustness. Particularly, the discrepancy between inversion results from the
shallow holes and the super-deep hole could be resolved by this technique. With the original code, the
inclusion of data from the SG-3 borehole leads to much worse fit with residuals of up to 1.5 K, and
minimum temperatures about 10 K below present values. Applying the GCV method, the inversion of the
SG-3 data yielded same result as obtained from the shallow holes: Moderate Weichselian temperatures of
4 K to 7 K lower than today.

Nonetheless, more experience with different data constellations are necessary, and a comparison with other
techniques is advisable, in particular the L-curve criterion (Farquharson and Oldenburg, 2004; Hansen
1992). The wide and multidisciplinary field of regularised inversions allows for further investigations into
better-adapted regularising operators which may imply more, and in particular better prior information on
GSTH behaviour. One possible candidate for this could be the minimum (gradient) support method (see
Portniaguine and Zhdanov, 1999; Zhdanov, 2002), or wavelet methods.

The goal of all of these efforts is to find the method which preserves best the information contained in
borehole temperatures. This thesis contributes to this endeavours by both demonstrating the significance
of permafrost in palaeotemperature inversions and by improving the methods.
LIST OF SYMBOLS

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<th>Symbol</th>
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<td>Smoothing operators (Tikhonov inversion)</td>
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<td>$c_p$</td>
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<tr>
<td>Symbol</td>
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<tr>
<td>$H$</td>
<td>Heat generation rate</td>
<td>W m$^{-3}$</td>
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<tr>
<td>$h$</td>
<td>Hydraulic head</td>
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<td>$H_f$</td>
<td>Fluid enthalpy</td>
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<tr>
<td>$K$</td>
<td>Hydraulic conductivity</td>
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<td>$L$</td>
<td>Specific latent heat</td>
<td>kJ kg$^{-1}$</td>
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<tr>
<td>$N$</td>
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<tr>
<td>$P$</td>
<td>Power</td>
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<td>$P_{acc}$</td>
<td>Acceptance probability (Monte Carlo inversion)</td>
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<tr>
<td>$Q$</td>
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<td>W</td>
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<tr>
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<td>W m$^{-2}$</td>
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<td>$S(p)$</td>
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<tr>
<td>$T$</td>
<td>Temperature</td>
<td>K, °C</td>
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<tr>
<td>$t$</td>
<td>Time</td>
<td>s</td>
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<tr>
<td>$T_S$</td>
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<td>Generalised cross validation function</td>
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<td>$v_a$</td>
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<td>m s$^{-1}$</td>
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<tr>
<td>$v_D$</td>
<td>Darcy velocity (specific discharge)</td>
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<td>$w$</td>
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<td>K</td>
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BIBLIOGRAPHY


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