UNCERTAINTY ANALYSIS AND INVERSION OF GEOTHERMAL CONDUCTIVE MODELS USING RANDOM SIMULATION METHODS

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Abstract

Knowledge of the thermal conditions in the lithosphere is based on theoretical models of heat transfer constrained by geological and geophysical data. The present dissertation focuses on the uncertainties of calculated temperature and heat flow density results and on how they depend on the uncertainties of thermal properties of rocks, as well as on the relevant boundary conditions. Due to the high number of variables involved in typical models, the random simulation technique was chosen as the applied tool for the analysis. Further, the random simulation technique was applied in inverse Monte Carlo solutions of geothermal models. In addition to modelling technique development, new measurements on thermal conductivity and diffusivity of middle and lower crustal rocks in elevated pressure and temperature were carried out.

In the uncertainty analysis it was found that a temperature uncertainty of 50 K at the Moho level, which is at a 50 km's depth in the layered model, is produced by an uncertainty of only 0.5 W m^{-1} K^{-1} in thermal conductivity values or 0.2 orders of magnitude uncertainty in heat production rate (μW m^{-3}). Similar uncertainties are obtained in Moho temperature, given that the lower boundary condition varies by ± 115 K in temperature (nominal value 1373 K) or ± 1.7 mW m^{-2} in mantle heat-flow density (nominal value 13.2 mW m^{-2}). Temperature and pressure dependencies of thermal conductivity are minor in comparison to the above mentioned effects.

The inversion results indicated that the Monte Carlo technique is a powerful tool in geothermal modelling. When only surface heat-flow density data are used as a fitting object, temperatures at the depth of 200 km can be inverted with an uncertainty of 120 - 170 K. When petrological temperature-depth (pressure) data on kimberlite-hosted mantle xenoliths were used also as a fitting object, the uncertainty was reduced to 60 - 130 K. The inversion does not remove the ambiguity of the models completely, but it reduces significantly the uncertainty of the temperature results.

Keywords: lithosphere, heat flow, thermal regime, Monte Carlo analysis

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Helsinki, March 2000 Jarkko Jokinen

List of the original articles

I Jokinen J & Kukkonen IT (1999a) Random modelling of the lithospheric thermal regime: forward simulations applied in uncertainty analysis. Tectonophysics 306 (3-4): 277–292.

II Kukkonen IT, Jokinen J & Seipold U (1999) Temperature and pressure dependencies of thermal transport properties of rocks: Implications for uncertainties in thermal lithosphere models and new laboratory measurements of high-grade rocks in the Central Fennoscandian Shield. Surveys in Geophysics 20: 33–59.

III Jokinen J and Kukkonen IT (1999b) Inverse simulation of the lithospheric thermal regime using the Monte Carlo method. Tectonophysics 306 (3-4): 293–310.

IV Jokinen J & Kukkonen IT (2000) Inverse Monte Carlo simulation of the lithospheric thermal regime in the Fennoscandian Shield using xenolith-derived mantle temperatures. Journal of Geodynamics 29: 71–85.

Contents

1. Introduction

The major aim of geothermal modelling is to present the internal temperature and heat-flow density distribution of a studied area. Temperature and heat transfer are involved in practically all geological and geophysical processes of the earth. For instance, when temperature decreases, melted rocks and minerals crystallize, the deformation of the rocks change from ductile to brittle, and the physical and chemical characteristics of geological materials vary accordingly. Actually, mantle convection and plate tectonics are expressions of heat transfer from the hot interior of the earth to its cool surface. It is this thermally driven system that initiates most of the fundamental geological processes and phenomena.

Our understanding of the internal thermal regime of the earth is based mainly on three factors: firstly, on direct measurements, secondly, on geological observations and thirdly, on geophysical modelling. The direct measurements include measuring drillhole temperatures, heat production rates of rocks and heat transport properties of rocks. Thermal transport property measurements are made in surface conditions, but also in elevated temperature and pressure conditions in specialized laboratories.

In this study, the attention is focused on geothermal models, their uncertainty analysis and inverse solutions. Traditionally, forward modelling has been used in geothermal studies. After deciding on the values of appropriate boundary conditions and thermal parameters, the temperature and heat flow values in the subsurface are calculated by solving the involved heat transfer equations, either analytically or numerically. However, the choice of parameter values usually involves considerable ambiguity, and the problem is further complicated by the related non-linearity, due to temperature and pressure dependencies of thermal conductivity of rocks, but often only one acceptable model is presented as a solution. Uncertainty analyses of forward models have rarely been discussed in geothermics.

Inverse solution, i.e. the combinations of parameter values and boundary conditions, can be mapped by the possible random solutions satisfying the measured data on temperature and heat-flow density. Inversion methods reduce the ‘personal bias’ sometimes involved in forward modelling, and may indicate solutions not apparent otherwise. Although inversion methods are commonly used in geophysics in general, their applications in lithospheric geothermics so far have been relatively few.

The reason for using the Monte Carlo (MC) method can be understood to be the ambiguity of geothermal models which in this respect is analogous to the travelling salesman's dilemma (Kirkpatrick et al. 1983). The task is to find the shortest route that visits all chosen sites and finally returns to the initial one. When this dilemma is converted into a mathematical form, the total sum of distances between the target sites is to be minimized. Using the simplest MC optimization, the solution can be found by selecting a set of random routes and then choosing the best of those. When the number of sites is small, the best route is determined by going systematically through all the possibilities. If the number of sites (n) is larger the number of different alternatives increases (n!) as well. Here the problem becomes more difficult because solving all possibilities is too slow and simply running through random models is not useful anymore. The one and only best route is no longer interesting in a case where many different routes have equivalent distances with insignificantly small differences. In further comparison, the search is made more efficient by using previous experience when guessing at new alternatives. Instead of indifferent allotment, the probability of a re-election of good subroute combinations is increased and respectively the probability of poor alternatives is decreased. In the travelling salesman's dilemma, sites close together have a high probability of becoming successive visiting sites on the route. The dilemma is thus divided into smaller 'subproblems' as happens also in the optimization of geophysical models. The most significant results are optimized first. When the changes in the model are no longer significant, the finishing of the process becomes possible. The visiting sites of the travelling salesman can be replaced by geothermal or whatever model parameters.

This dissertation is based on four independent publications given in the appendix, and containing the original contributions to applying MC methods in uncertainty analyses (papers I and II) and inverse solutions (papers III and IV). The dissertation synopsis first summarizes the general theory of heat transfer in a geological medium (Chapter 2) and then discusses the MC method in the framework of general inversions as well as global optimization methods (Chapter 3). In Chapter 4, the structure of the simulations in papers I–IV is presented. The major results of the independent publications are summarized in Chapter 5 and 6.

2. Heat transfer

Thermal energy is transferred in the geological medium towards a lower temperature by lattice conduction, convection or radiation. In addition to temperature difference, thermal conductivity is an important factor controlling conductive heat flow. Further, in transient heat flow problems, thermal diffusivity (or density and specific heat capacity) is a relevant parameter. Due to the temperature dependence of lattice phonon conduction, both thermal conductivity and diffusivity decrease with increasing temperature. Convective heat transfer is controlled on the one hand by the driving forces (buoyancy) produced by density differences due to heat expansion of viscous rock or pore fluid (free convection in the mantle or in an aquifer) or, on the other, by pressure gradients due to topographically controlled variations in the ground water table (advection or forced convection). In addition to these, hydraulic permeability is an important material property controlling flow velocities. Radiative heat transfer is dependent on temperature according to the Stefan-Bolzman law. In geological media, opacity is the critical property of the rocks controlling the efficiency of radiation. In the following, the major heat transport mechanisms are shortly discussed.

2.1. Conductive heat transfer

The conduction of heat can be presented by Fourier's first law (Haenel *et al*. 1988), which has been derived experimentally:

$$Q = -\frac{l\left(T_2 - T_1\right)}{h}, \tag{1}$$

where Q is the quantity of heat [J], λ is thermal conductivity [W m^{-1} K^{-1}], $T_2 - T_1$ is temperature difference [K] between the two boundary surfaces of a plano parallel plate, A is the surface area of the plates [m^2], t is the time [s] during which the heat flows and h is the thickness of the plate [m]. The heat-flow density q for unit area and unit time is

$$q = -l\,\frac{dT}{dh}. \tag{2}$$

This is also the basic equation to be used to determine geothermal heat-flow density in boreholes with temperature measurements at different depths for gradient estimation, and also in the corresponding laboratory measurements of thermal conductivity from the samples. Generally, heat flow is three dimensional

$$\mathbf{q} = -l\nabla T = -l\,grad T \tag{3}$$

where q [W m^{-2}] and temperature gradient ∇T are vectors (q = (q_x, q_y, q_z), ∇T = ∂T / ∂x + ∂T / ∂y + ∂T / ∂z). The commonly needed differential operators are the Hamilton-operator (Nabla) and the Laplace-operator, marked: ∇ = (∂ / ∂x, ∂ / ∂y, ∂ / ∂z) and respectively Δ = ∇·∇ = (∂^2 / ∂x^2 + ∂^2 / ∂y^2 + ∂^2 / ∂z^2).

Thermal energy flowing through the volume dV (dx dy dz) in unit time is marked

$$P_{flow} = -\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right) dV \tag{4}$$

where P is power [W] and the vertical heat-flow density dq_z through the plate dx dy is -(∂q_z / ∂z) dV and dq_x, dq_y respectively.

Independently of the previous equation, thermal energy flow P to the volume element dV during unit time can be solved by equation

$$P_{stored} = rc dV \frac{\partial T}{\partial t}, \tag{5}$$

where ρ is the density [kg m^{-3}], c is specific heat capacity [J kg^{-1} K^{-1}], (ρc is volumetric heat capacity), dV is the volume [m^3], and ∂T / ∂t is the temperature change during unit time t [s].

Fourier's second equation is developed by setting (4) and (5) equal (Haenel at al., 1988)

$$-div(\mathbf{q}) = rc\frac{\partial T}{\partial t}. \tag{6}$$

Substituting for q with corresponding equations:

$$\left[\frac{\partial\left(l_x \frac{\partial T}{\partial x}\right)}{\partial x} + \frac{\partial\left(l_y \frac{\partial T}{\partial y}\right)}{\partial y} + \frac{\partial\left(l_z \frac{\partial T}{\partial z}\right)}{\partial z}\right] = rc\frac{\partial T}{\partial t} \tag{7}$$

and then assuming the rock material to be isotropic and homogeneous (λ_x = λ_y = λ_z = λ), it follows that

$$\frac{\partial T}{\partial t} = \frac{l}{rc}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right) = a\Delta T\ , \tag{8}$$

where a (= λ / ρc) is thermal diffusivity [m^2 s^{-1}]. According to equation (8), a time-dependent temperature change (moving of the temperature pulse) is controlled by thermal diffusivity.

Given that there is an internal heat generation in the medium, a new term is added

$$\frac{\partial T}{\partial t} = a\Delta T + \frac{H}{rc} \ , \tag{9}$$

where H is heat production rate [W m^{-3}]. The temperature varies as a function of conductive heat transport and heat production (or heat sink). Heat production of rocks in the crust is primarily caused by radioactive elements, but may be present also due to mineral reactions during diagenesis and metamorphism. In a steady state condition ($\partial T / \partial t = 0$) equation (9) is called the Poisson-equation ($a \Delta T + H / \rho c = 0$) and with no heat production the rest of the formula is called the Laplace-equation ($\Delta T = 0$).

The most common sources of radiogenic heat production are natural radioactive isotopes of uranium (the decay series of ^{238}U and ^{235}U), thorium (^{232}Th), and potassium (^{40}K) (Buntebarth, 1984; Rybach, 1988). Heat production in rocks can be calculated as

$$H = r\left(9.52c_U + 2.56c_{Th} + 3.48c_K\right)10^{-5} \ , \tag{10}$$

where H is heat production rate [$\mu W\ m^{-3}$], ρ is density [kg m^{-3}] and c is the total concentration in ppm (parts per million) [10^{-6} kg kg^{-1}] for uranium and thorium, and % for potassium. The ^{40}K / K ratio is assumed to be constant. Numerical values in the equation (10) are the heat production constants H [W kg^{-1}] of the decay series of uranium, thorium, and potassium.

Analytical solutions such as equation (9) have been widely used in geothermics. The most common types of problems are those where the equation is solved as a boundary value problem with known surface temperature and mantle heat-flow density (see, e.g. Carslaw & Jaeger (1959) for a wealth of solutions).

Temperature within a layer with constant conductivity and heat production is calculated as follows (Turcotte & Schubert, 1982). Firstly, the total increase of the heat flow of thin (infinitesimal) slab depends on the heat production rate (per unit mass) H, on density ρ and the thickness of the slab δz. Secondly, the change of heat flow in the thin slab depends on the thickness of the slab and on the rate of change of the heat-flow density. Fourier's law (equations 1 and 2) has been used as Turcotte & Schubert (1982) have been presented. When we equalize these to describe the changing rate of the heat-flow density, we obtain

$$rHdz = dz\left(-l\left(\frac{d^2T}{dz^2}\right)\right) \tag{11}$$

and further

$$rH = -l\,\frac{d^2T}{dz^2} \ . \tag{12}$$

At the surface of a half-space z = 0, the temperature is T_0 and heat-flow density is q_0 . The first constant of the integration is $c_1 = q = -q_0$ [W m^{-2}] and the second constant of the integration is $c_2 = \lambda\, T = \lambda\, T_0$ [W m^{-1}] on z = 0. The first integration of the equation (12) gives

$$rHz = -l\,\frac{dT}{dz} + q_0 \tag{13}$$

and the second integration results

$$rH\,\frac{z^2}{2} = -lT + q_0 z + lT_0. \tag{14}$$

Finally, the temperature at the depth z is

$$T = T_0 + \frac{q_0}{l}\,z - \frac{rH}{2l}\,z^2, \tag{15}$$

where T_0 is the surface temperature, q_0 is the surface heat flow density, ë is the thermal conductivity and H is the heat production rate.

It is common to assume that heat production decreases with depth because the mafic low heat production rocks become more common with depth (Heier & Adams, 1965). For such cases there are different possible solutions. The equation (15) can be applied to layer models by calculating temperatures consecutively layer by layer with different heat production values from top to bottom. Alternatively, the heat production rate at the depth z [m] can be described for instance as $H(z) = H_0 \exp(-z / d)$, where d is the particular distance [m] at which heat production is reduced to the value 1 / e (= 0.368) of its value at the top boundary (Buntebarth, 1984). Then, the solution of the equation (9) is of the form:

$$T(z) = T_0 + z\,\frac{q_0}{l} - z\,\frac{H_0 d}{l}\exp\left(-\frac{h}{d}\right) + \frac{H_0 d^2}{l}\left(1 - \exp\left(-\frac{z}{d}\right)\right), \tag{16}$$

where h is the thickness of the layer. The solutions become more complex if the temperature dependence of the thermal conductivity is included. Such results have been compiled e.g. by Čermák & Haenel (1988).

2.2. Convective heat transfer

Flowing water transfers heat to and from the rock depending on the temperature difference between those two (Haenel *et al*., 1988). The heat transported by water flow is

$$q = div\left(r_w c_w v_f T\right), \tag{17}$$

where q is heat-flow density [W m^{-2}], ρ is density [kg m^{-3}], c is specific heat capacity [J kg^{-1} K^{-1}], v_f is the Darcy velocity of fluid in a porous medium [m s^{-1}] and T is temperature [K]. The index w refers to water and the index f to filtration. The so-called Darcy velocity (or pore velocity) is: $v_f = v_a$ P, where v_a is the average velocity of the (water) particle [m s^{-1}], and P is the porosity of the medium [%]. The originally experimentally determined Darcy's law is given by

$$v_f = k_f\,gradh\,, \tag{18}$$

where k_f is the hydraulic conductivity [m s^{-1}], the subscript f refers to flow and grad h stands for dimensionless hydraulic pressure gradient (water-level differences [m] / horizontal distance [m]).

In a homogeneous and isotropic medium the equation (9) of heat transport will be completed by the convective part:

$$\rho_A c_A \frac{\partial T}{\partial t} = \lambda_A \Delta T + H - div(\rho_w c_w v_a T), \tag{19}$$

where the subscript A refers to the average values of the medium – including the properties of rock and water in a saturated medium. The properties of rock, fluid, and medium are related:

$$\lambda_A = (1-P)\lambda_r + P\lambda_w \tag{20}$$

and

$$\rho_A c_A = (1-P)\rho_r c_r + P\rho_w c_w, \tag{21}$$

where P is the porosity [%], r refers to rock and w refers to water (or gas).

These equations for hydrological problems can be simplified in large scale problems such as lithosphere geothermics. However, hydrology may have an important role in affecting heat-flow density in drill holes (Smith & Chapman, 1983) and all disturbances should be carefully removed from the data before applying them to conductive models. Both temperature and heat-flow density are predisposed to errors owing to water flow in the drill holes and climatic changes that have taken place over time. These phenomena and their effects on the Fennoscandian Shield have been discussed for example by Jõeleht and Kukkonen (1996), Kukkonen (1988, 1995), Kukkonen & Clauser (1994), Kukkonen *et al.* (1998), and Balling (1995). Hydrological corrections in thermal models can be solved also by applying pure hydrological models like Bear & Verruijt (1987) have shown.

2.3. Thermal conductivity

Because of the temperature and pressure dependence of thermal conductivity, the heat conduction equation is a non-linear problem. A typical equation used for temperature dependence of lattice (phonon) thermal conductivity is

$$\lambda = \frac{1}{A + BT}, \tag{22}$$

where A [W^{-1} m K] and B [W^{-1} m] are constants related to the scattering properties of phonons. According to Schatz & Simmons (1972) A is related to the scattering of phonons by impurities and imperfections, and B is related to phonon-phonon scattering.

Radiative heat transport follows the T^3 -law where T = T [K]. In rocks, radiative transport becomes relevant at about 1000 K. Combining lattice and radiative heat transfer into one conductivity value yields

$$l = \frac{1}{A + BT} + CT^3, \tag{23}$$

where C [W m^{-1} K^{-4}] is a constant controlled by the refraction and extinction properties of the matter (Schatz & Simmons, 1972). Due to several involved factors, laboratory experiments of thermal conductivity at high temperatures can alternatively be fitted with many other types of formulas than the two previous equations (Hanley *et al.*, 1978; Kukkonen & Jõeleht, 1996; Lehmann *et al.*, 1998). Laboratory measurements have been conducted and collected among others by Balling (1976), Clauser (1988), Clauser & Huenges (1993), and Zoth & Haenel (1988). The data presented in the literature indicates that common rock types show more or less similar temperature dependent behaviour even though results from individual minerals can be very different and strongly influenced by anisotropy (Clauser, 1988; Clauser & Huenges, 1993). Generally, thermal conductivity of quartz-rich rocks decreases more rapidly with temperature than that of quartz-poor rocks.

Seipold (1998) compiled the presently available data on temperature dependencies of thermal conductivities of different rock types fitted to the equation (22). Since it is difficult to see the connection between the parameters A, B, and the measured conductivity values at elevated temperatures, a practical formulation of equation (22) is introduced below. Instead of using parameters A and B, it is possible to use two other parameters, namely thermal conductivity at a reference temperature λ_0 [W m^{-1} K^{-1}] and the single temperature coefficient of thermal conductivity b [K^{-1}]. The values for λ_0 and b can be formed by equating

$$\frac{1}{A + BT} = l_0 \frac{a}{1 + bT} \tag{24}$$

and by including the solution in the reference temperature: $\lambda_0 = 1 / (A + B\ T_0)$ which results in $a = 1 + b\ T_0$ and b = B / A, where T = T [K] and T_0 = 293 K = 20 °C (for instance). Joining the parameters a and b leads to the following form of temperature dependence of λ

$$l = l_0 \frac{1 + bT_0}{1 + bT}. \tag{25}$$

Respectively, transformations in the opposite direction are $A = (\lambda_0 (1 + b\ T_0))^{-1}$ and B = b A. equations (25) and (22) give identical temperature dependences of thermal conductivity. The benefit of using eq. (25) was clearly seen in the uncertainty analysis because pure temperature dependence could be simulated with only one parameter.

Table 1. Parameters A, B, b, and λ_0 of temperature dependence of thermal conductivity after Seipold (1998) and Kukkonen et al. (1999). Mafic granulites I are from the Kiuruvesi area and mafic granulites II are from the Varpaisjärvi area, both in Finland (paper II). Calculated $b = B / A$ and $\lambda_0 = 1 / (A + B T_0)$, where T_0 is the reference temperature 293 K (20 °C). N is the number of samples.

	A	B*10000	b*1000	λ_0	N
Amphibolites	0.375	1.89	0.504	2.32	16
Basalts	0.359	1.43	0.398	2.49	4
Granites	0.203	4.07	2.005	3.10	15
Granulites	0.271	3.66	1.351	2.64	8
Gneisses	0.241	3.48	1.444	2.92	26
Pyroxenites	0.375	1.89	0.504	2.32	16
Serpentinites	0.427	1.10	0.258	2.18	7
Olivine rocks	0.110	3.18	2.891	4.92	13
Mafic granulites I	0.417	1.8	0.432	2.13	3
Mafic granulites II	0.440	1.04	0.236	2.13	5

As shown by Seipold (1998) the parameters A and B are correlated, and consequently also λ_0 and b. On the basis of table 1 and fig. 1, the coefficient of temperature dependence of thermal conductivity b increases (on the average) with an increase of thermal conductivity in the reference temperature λ_0. Typically, phonon conductivity decreases with increasing temperature asymptotically towards the value of 1 - 2 W m^{-1} K^{-1}. This fact is useful in case of missing data or poor knowledge about the rock type.

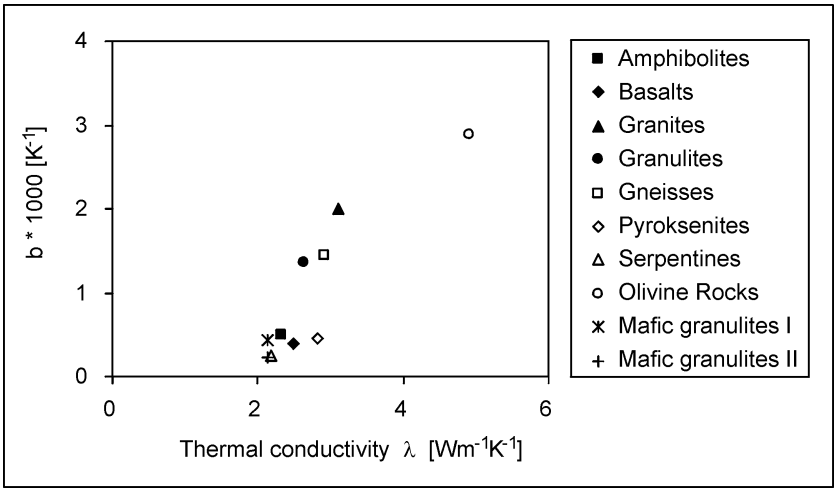

Fig. 1. Correlation between coefficient b (temperature dependence of thermal conductivity) and thermal conductivity λ_0 in room temperature.

The influence of pressure on thermal conductivity consists of two phenomena. Below a pressure value of about 100 MPa, the effect of microcracks gradually disappears with increasing pressure (Buntebarth 1984). Due to this compression, thermal conductivity rises rapidly to a more stable level. This threshold change in thermal conductivity as well as in thermal diffusivity (Seipold 1995) can be up to several tens of percent, depending on the porosity properties of the rocks. At depths greater than c. 3.4 kilometres (c. 100 MPa), the pressure dependence of thermal conductivity increases approximately linearly with the rising pressure due to the reduction in the intrinsic porosity and the compressibility of rock-forming minerals. The increase in the thermal conductivity of granite is typically about 12 % GPa^{-1} (1 GPa corresponds to the depth of c. 34 km in the earth's crust) (Seipold 1995), but much smaller values are reported as well, e.g. in the new data on the mafic high-grade rocks in paper II. The pressure dependence of thermal conductivity follows the function $\lambda = \lambda_0 (1 + a\ p)$, where a is the coefficient for the pressure dependence of thermal conductivity [Pa^{-1}] and p is the pressure [Pa].

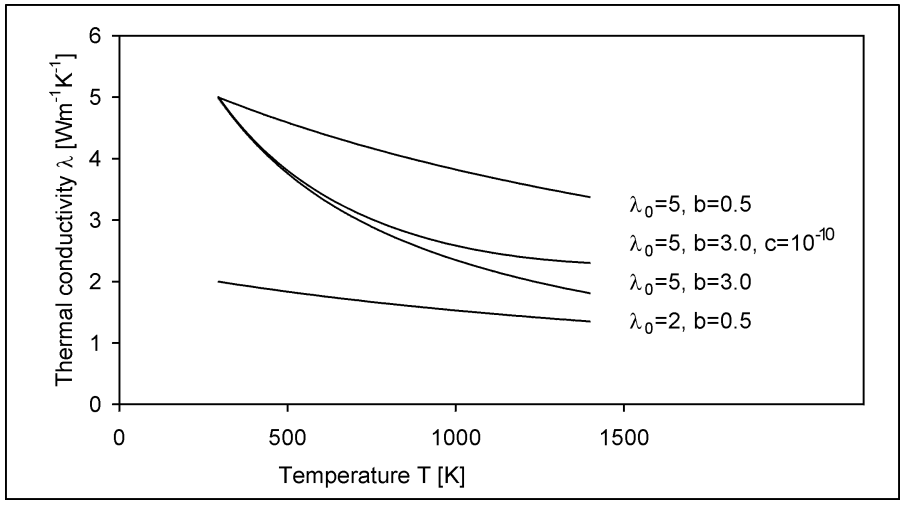

Fig. 2. Four examples on temperature dependence of thermal conductivity calculated using equation (25).

3. Introduction to the Monte Carlo simulation and related methods

Geophysical inversion methods can be divided into direct inversion and model based inversion methods (Sen & Stoffa 1995) (table 2). Direct inversion is feasible only in very few applications and the majority of inversion methods are model based. Problems, characterized by linear correlations of model parameters and measured data or which can be linearized into such, can be inverted using the linear, iterative linear, and gradient methods. These methods may not be very useful in problems with a high degree of non-uniqueness and a large number of involved parameters. This is typical of geothermal problems with poorly constrained conductivity and heat production variations in the lithospheric scale divided in numerous geometric domains. The ambiguity of the problem can be mapped with exhaustive grid search methods, i.e. testing each possible model to find the acceptable inversion solutions. However, in large models this leads to very high numbers of models and even with reasonable numbers of discrete parameter values the method is not feasible.

Table 2. Inversion methods in geophysics (Sen & Stoffa 1995).

Direct inversion methods
Model based inversion methods
Linear and linearized methods
Iterative linear or gradient based methods
Enumerative or grid search methods
Monte Carlo methods
Directed Monte Carlo methods
Global optimization methods
Simulated annealing methods
Metropolis algorithm
Genetic algorithm

For non-linear, non-unique problems with large numbers of involved model parameters, Monte Carlo (MC) methods and directed MC methods are interesting alternatives. In this work MC methods were applied in geothermal lithosphere modelling.

The MC inversion method consists of using a pseudo-random number generator to generate models in a priori model space, of computing a forward solution for each model and using some qualitative criteria for comparison between measured and modelled data to decide which new models are acceptable a posteriori models (Press 1968, Tarantola 1987). Reliability (randomness) of evenly distributed random numbers (Binder & Stauffer 1984) is a prerequisite in MC applications. It ensures, that the generated models consist of different but statistically equivalent parameter combinations. A reliable response is important from a statistical standpoint but especially in uncertainty and sensitivity analyses.

MC simulation has been used in geophysics with increasing interest, and not only because of the constantly improving efficiency of computers. Recently, a key-paper was given by Mosegaard & Tarantola (1995) who presented the general principles of applying MC sampling in geophysical inverse problems with an application to gravity interpretation. The earliest known geoscientific application of MC inversion was made by Press (1968) who modelled the travel times of compressional and shear waves, and the mass and moment of inertia of the earth in order to solve velocity and density distribution of the earth. An early geothermal application of the MC method was given by Čermák (1971) who studied ground temperature histories at borehole sites. Past ground temperatures were also studied with the MC method by Dahl-Jensen *et al*. (1998) in the Greenland ice sheet. Royer & Danis (1988) applied random variation to the mantle heat flow and calculated confidence intervals for the thermal field. Lamontagne & Ranalli (1996) studied the effects of uncertainty of thermal parameters on the rheological properties of a seismically active area.

Other interesting geothermal and hydraulic inversion studies have been presented by Wang (1989), Wang & Beck (1989), and Lehmann *et al*. (1998), who utilized the Bayesian parameters estimation method in lithosphere models and the German KTB super-deep hole case. Kolditz & Clauser (1998) presented a ‘deterministic fracture network approach’ in their 3D heat and fluid transport simulation in hot dry rock applications. Their method is intermediate between deterministic and stochastic simulation methods.

An essential feature of the MC simulation is that it is dealing all the time with probabilities. In the beginning of the simulation there is a broad model space where also the best model configuration has an equal possibility to all other models. In the simulation, the variation possibilities of the model parameters concentrate near the optimal solution, i.e. the most probable parameter combinations are gaining weight in the probability function within the model space.

The MC inversion consists of several, often deeply interrelated stages. The random walk and parameter sampling are associated with the model generation in the a priori model space. Model acceptance is the most essential part of a simple MC inversion in particular. It is like a gateway between the a priori and a posteriori model spaces. The annealing process / cooling schedule is involved in the directed MC simulation, where a previous a posteriori solution or other non-uniform probability density function directs

the variation possibilities of the random models during the optimization process. The grounds for these expansions of simple MC simulations as well as for the parameter sampling and random walk are introduced in the following chapters.

3.1. Parameter sampling

Solving a geothermal model with the MC method is a stochastic process which in this work has been realized in a stationary way. In parameter sampling all blocks (lithological units) in the model are given a random parameter value from the established probability density functions (pdf). Alternatively, a stochastic process can be built for example by following the Markow process, Kriging sampling or Gaussian simulation process, where the block properties are dependent on a certain distance between each other and where the selected model blocks can represent initial points. A random model generated through a stochastic process is called a stochastic realization. The meaningfulness of such simulations requires that representative data on the autocorrelation of thermal properties, i.e. a variogram analysis on real data, is available (Deutsch & Journel 1998). For instance, in the doctoral theses of Niemi (1994) and Laine (1998), the variogram analysis forming part of the parameter sampling was conducted using the realistic data. In this work, the correlation between the properties of model blocks has not been used owing to the lack of knowledge on the spatial continuity of thermal model parameters in the lithospheric scale.

In geologically homogeneous rock units, distributions of geothermal parameters are narrower than they are on the average in combinations of lithological rock groups in general, as shown in paper I and by Peltoniemi & Kukkonen (1997). In modelling this leads to the fact that larger domains involve greater uncertainties than do more restricted ones, as small domains 'include' less heterogeneity than larger ones. A typical dimension of a small model block in a geophysical numerical lithosphere model is about 10 km. Here, parameter variations may be very broad due to normal geological heterogeneity. On the other hand, the most extreme measured parameter values of typical laboratory samples (diameter less than 10 cm) from a study site are often not representative of typical rocks in the area. There is a small possibility that such rocks and their properties are predominant deeper in the subsurface. For instance, such a case was investigated in a gravity study in Central Finland where mafic dioritic and gabbroic rock types are a minority in outcrops at the surface, but gravity models require that such rocks are very common at greater depths (Jokinen 1997). On the basis of these facts, parameter distributions have been defined loosely in such a way that also rarely observed data values have at least a small possibility to be selected as an average value of a block in the MC model.

In the lithospheric thermal models, thermal conductivity λ and heat production rate A are the most important rock parameters. All four companion papers in this work apply λ and A of the Baltic-SKJ model of Kukkonen & Joeleht (1996), who compiled the values using seismic velocities, Poisson ratios, lithological interpretation, geochemical data on outcrops, as well as literature information on the middle and lower crustal rock types. Also the data presented by Peltoniemi & Kukkonen (1997), Čermák & Rybach (1982), and Zoth & Haenel (1988) has been used to define the pdf for different model blocks. On

the basis of the analysis of the Finnish data set by Peltoniemi & Kukkonen (1997), the heat production A of individual rock types is most often either normally distributed or log-normally distributed. Since the distribution of all heat production samples in the study of Peltoniemi & Kukkonen (1997) is close to a log-normal distribution (paper I), the log-normal distribution type was used for the heat production of all rock types in the MC simulations. On the other hand, a normal distribution was used for thermal conductivity. Uniform distributions with loose constraints have been used in paper III and paper IV, where a relatively conservative assumption was considered best due to the involved ambiguity.

Generating pseudo-random numbers is usually realized with reliable computer codes such as those given by Abramowitz & Stegun (1972) and Press *et al*. (1990). The transformation of a uniformly distributed random number into a representative sample of the Gaussian distribution is achieved using the Box-Muller method utilizing trigonometric functions (Press *et al*. 1990).

The Gaussian distribution function is

$$F(x) = \int_{-\infty}^{x} dx'\, p(x') = \tfrac{1}{2} + erf\left(\frac{x-\bar{x}}{s}\right), \tag{26}$$

where erf(x) is the error function (Abramowitz & Stegun 1972), σ is the standard error of the parameter x (σ^2 is the variance of the parameter x) and is the average of the parameter (expectation value). Classified normal distribution can be developed by the Box-Muller method (Press *et al*. 1990) in practice. The probability density function of a normal distribution is

$$p(x) = \frac{1}{s\sqrt{2p}} \exp^{-\frac{1}{2}\left(\frac{x-\bar{x}}{s}\right)}. \tag{27}$$

Parameter sampling can be accomplished either to achieve directly a continuous variable distribution, or discretely using a predetermined biassing difference and selected number of classes (or limits). However, the discretization of the distribution in the simulation process is needed only in analysing the obtained a posteriori distributions.

3.2. Annealing process

The term ‘annealing’ has been developed from a metallurgical process where melted steel is cooled under careful thermal control. The term has been adopted into mathematical terminology for better visualization of certain optimization techniques. An annealing process is a development where the accepting conditions of random models are slowly tightened in such a way that the tightening process takes place slowly enough in relation to the number of tested models. Annealing methods differ from one another in how the accepting conditions are tightened, how additional detail is reached in a model solution, and how the stabilization of a posteriori model space is pointed out (or sometimes avoided). The speed of annealing is controlled / predetermined by a ‘Cooling Schedule’.

There are two important concepts in the simulated annealing method, namely, thermodynamic temperature (T) and energy (E), which are controlled and observed during the simulation (Kirkpatrick *et al*. 1983, Sen & Stoffa 1995). Temperature, in this case, has nothing to do with the rock temperature in thermal models. Thermodynamical temperature (T) is associated with the limitations of the a posteriori model space. Shortly defined, it expresses the acceptable value of noise variance (the misfit function). When the temperature is high, a priori model parameters can vary very loosely and models are accepted quite easily into the a posteriori distribution. Temperature as an acceptance statement is tightened (the model is annealed) during the simulation. New models have to yield on an average smaller residuals between calculated and observed values than the old ones in order to be accepted directly to the a posteriori distribution. The energy (E) is associated with one model. It measures the difference between the solution of one random model and observations, i.e. the value of the misfit function. The error of each individual model is related to the accepted variation possibilities of the model parameters. With the a priori distributions having large standard deviations the model's energy can be high: the misfit between accepted models and measurements is large. The aim of MC inversion is to map those possible acceptable models and their parameter distributions that are the most probable solutions of the inverse problem within the limits of the given thermodynamic temperature and energy.

At the end of a completed annealing process when the thermodynamic temperature is zero there is only one model (or a number equally good models) left that gives the best solution with respect to the optimized result (the global minimum of error function). In such a case a deterministic solution is obtained using an originally stochastic starting point.

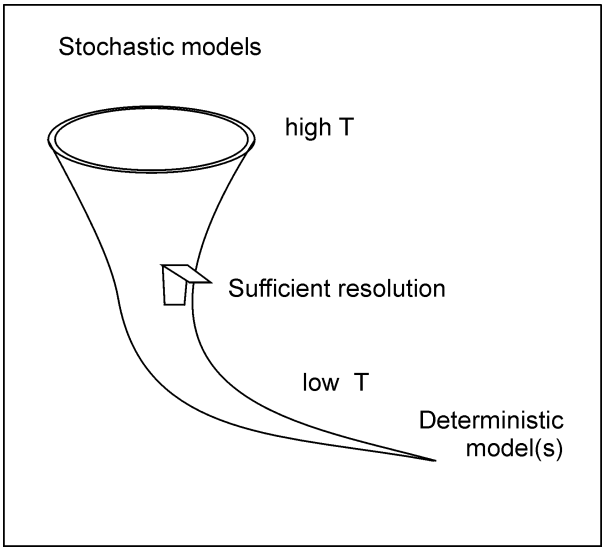

Fig. 3. Symbolic presentation of simulated annealing.

Symbolically, simulated annealing can be described as a narrowing tube or tunnel. The diameter of the tunnel (fig. 3) corresponds to both the temperature and energy of the models and is controlled by the annealing process. The length (elevation) of the tunnel reflects the chronology of the process. It may include a number of thresholds and cooling stages where the requirements of equilibrium of results and of model parameter distributions have been met. Each threshold represents a decrease in thermodynamic temperature. The annealing process can be interrupted when reasonable resolution of solution has been reached (the door in fig. 3), otherwise no improvements in parameter distributions are achieved although temperature is decreased. In a very simple model the door may be closed with respect to a deterministic solution, and with truly ambiguous models the simulation expires already close to the initial state. A well designed SA process produces an efficiently narrowing tunnel (fig. 3), where the number of different acceptable models is rapidly reduced and the deterministic solution is near. If the thermodynamic temperature is too tight at the beginning, only the local minimum instead of the global minimum of the error function may be found (Kirkpatrick *et al*. 1983, Sen & Stoffa 1995). An illustrative example about a well designed SA process (in electromagnetic modelling) has been given by Sharma & Kaikkonen (1998).

Since geophysical models can be constructed in very different ways, the appropriate annealing process has to be tailored for each problem and case individually. The fact how deep down it is possible to proceed in annealing is controlled by the acceptable value of the thermodynamic temperature in the studied problem. In other words, the noise level of measurements is critical. In geothermics HFD measurements form this particular data. Unfortunately, HFD data show large variation and the simulation will be interrupted quite early on.

A proper simulation process provides statistically enough data during annealing and the model space is covered sufficiently. Sen & Stoffa (1995) recommend a method presented by Kennett & Nolet (1978) where the sufficient number of data samples is determined using the stabilization of resolution matrices calculated from changes in the parameters' mean values. Solved covariance and correlation matrices have been used to estimate uncertainties in the mean model parameters and correlations between the model parameters in the VLF inversions by Sharma & Kaikkonen (1998) and Kaikkonen & Sharma (1998). A similar technique has been used also in the works of Lehmann *et al*. (1998) and Wang & Beck (1989). In uncertainty analysis this is an appropriate method. However, thorough testing of the equilibrium of the a posteriori parameter distributions would be for example the χ^2-test.

3.3. Metropolis algorithm

The Metropolis algorithm (Metropolis & Ulam 1949, Metropolis *et al*. 1953) is reliable SA optimization method. The characteristic idea in the Metropolis algorithm is the 'random walk' in the a priori model space and the use of a conditional clause for accepting models into the a posteriori model space. This 'Metropolis rule' (Mosegaard & Tarantola 1995) will be described in the following equations. The Metropolis algorithm is applied in the companion papers III and IV.

In the Metropolis algorithm, the previous model is changed only slightly, and depending on the obtained result, the model is either accepted or rejected. The length of the shortest step in the random walk equals exactly one biassing difference in the distribution of a single parameter (in a discrete a priori model space) and its both possible directions have equal probabilities (Sen & Stoffa 1995). In each application, the random walk has to be tailored independently.

Between the solution of the simulated model and the observed result a value of the probability function L(m) (Mosegaard & Tarantola 1995) is calculated

$$L(m) = k \exp\left(-\frac{E(m)}{T} \right), \tag{28}$$

where k is a constant, T is the thermodynamic temperature and, following Mosegaard & Tarantola (1995), the energy E of the model m is identified as the misfit function

$$E(m) = \tfrac{1}{2} \sum_{i=1}^{N} \left(g(model)_i - g(data)_i \right)^2 , \tag{29}$$

where g is the result vector of the model or data. Mosegaard & Tarantola (1995) have defined T in the form of s^2 and it is called the total 'noise' variance. The value of the probability function is compared with the corresponding value of the previous model. If the model is equal or better than the previous one (i.e. the E(m) is smaller: $\Delta E = E_{old} - E_{new} \leq 0$) it will be accepted as a sample into the a posteriori group. However, if the value is higher the model may still be accepted. The probability limit is calculated as follows

$$p(accept) = \exp\left(\frac{-\Delta E}{s^2} \right), \tag{30}$$

where ΔE is the difference of error functions between the comparison model and the random model. A random number [0,1] will be compared with P. When the random model is very near the accepted model, P is close to 1 and accepting probability is quite high. If the random number is higher than P the new model will be rejected and the previous model will be accepted to the a posteriori distribution again. Further, a new model is drawn and its energy value is compared to the energy of the latest accepted model added to the a posteriori space according to the previous equations.

Good models are not replaced quickly in the process and therefore they are stacked repeatedly in the a posteriori group. Respectively, worse models are quickly replaced by better models and thus they are not significant in the a posteriori space.

The efficiency of the Metropolis algorithm in practice depends on how the random walk has been designed. A step from the accepted model to the next random model has to be appropriate – not too long or not too short. Otherwise the good property of the model disappears too quickly (long step), or the model is dependent on neighbouring models (short steps), i.e. they are too similar. The mutual dependence of models represents a serious dilemma in non-unique problems, i.e. the statistical interdependence of the accepted a posteriori samples. The interdependence of models can be investigated using the autocorrelation of the probability function as Mosegaard & Tarantola (1995) have suggested. In their gravity application, at least a hundred small steps had to be taken before the new model was statistically independent of previous models. When the sum of

many small changes is appropriate the characteristics of an accepted model are repeated in the next models and, similarly, because of the random accepting condition there is still a possibility to escape the local minimum of the misfit function.

When the a posteriori distribution of the simulation is stabilized, the probability P at the temperature T and with the energy E_i follows the Gibbs-Bolzmann distribution

$$p_i = \frac{\exp\left(-\frac{E_i}{T}\right)}{\sum_j \exp\left(-\frac{E_j}{T}\right)}, \tag{31}$$

where energy is associated with the i-th point in the configuration space and j = 1, N where N is the number of parameter combinations (Mosegaard & Tarantola 1995). The probability is independent of the a priori distribution.

3.4. Random walk algorithms

Parameter sampling is connected to one variable of the model, but random walk is associated rather with the whole model space. An effective SA process can be reached by making the guided random sampling from a continually revised pdf which is closer to the a posteriori distribution than for instance a uniform distribution would be. In this sense, a better SA algorithm than the classical Metropolis algorithm is provided e.g. by the Heat bath algorithm (Rebbi 1984), Fast simulated annealing algorithm (Ingber 1989), Simulated annealing without rejected moves (Greene & Supowit 1986), or the Mean field annealing algorithm (Peterson & Anderson 1987).

In the Heat bath algorithm (Rebbi 1984, Sen & Stoffa 1995) the random walk used is a combination of exhaustive search and a random selection process. Each parameter is varied through all possible different discrete values, while all other model parameters are kept simultaneously constant. Good solutions yield the varied parameter's pdf further providing a step in the random walk for the next model.

Simulated annealing without rejected moves (Greene & Supowit 1986, Sen & Stoffa 1995) attempts to reduce the number of models needed in the simulation. Parameter sampling is directed simultaneously to every parameter. The pdf of each model parameter is changed due to energy produced and next model is drawn from the updated pdf.

Fast simulated annealing (FSA) (Ingber 1989, Sen & Stoffa 1995, Szu & Harley 1987) is quite similar to the classical Metropolis algorithm. However, instead of a uniform distribution a Cauchy-like distribution is used in the FSA method. The new model is selected near the previous model. This again creates better accepting relations (ergodic SA improvement) in comparison to the Metropolis algorithm.

Ingber (1989) introduced both the Very fast simulated annealing (VFSA) and Very fast simulated reannealing (VFSR) methods. In these methods the accepting temperature is changed according to the sensitivity of an optimized parameter. Also the step length of the random walk is varied during the simulation process. Annealing and the random walk interact, and the cooling schedule is not easy to define either. In the VFSR method the major differences in comparison to the VFSA method are associated with the cooling

schedule, which makes it possible to anneal different parameters separately. An application of the VFSA method has been used recently by Sharma & Kaikkonen (1998) in the inversion of VLF and VLF-R data.

In the Mean field annealing (MFA) method (Peterson & Anderson 1987, Sen & Stoffa 1995) model parameter distributions are formed to resemble neural networks. The MFA method still is close to the other SA methods, but it differs in that the MFA method simulates brain and neuron activities. Parameter pdfs are no longer independent but interconnected. In a successful model the dependence between the used parameter values (synaptic strengths) is increased with a certain weight value and correspondingly, in a failing model, model dependence between the used parameter pdf values is weakened. A step of the random walk is always dependent on the current parameter configuration in the model space.

3.5. Cooling schedule

When finishing a sufficiently long random walk the temperature of the model will be decreased (the model is annealed). Annealing implies that the variation possibilities of approved solutions become limited and possibly the step length can be shortened. By using a shorter random walk step the results become more detailed (Sen & Stoffa 1995). The applied cooling schedule determines the next acceptance limits (noise variance) when the equilibrium of parameter distributions has been reached.

In the Metropolis algorithm, a cooling schedule can be formed exponentially according to the following function (Kirkpatrick *et al*. 1983) or by presenting a corresponding, more accurate, problem specific algorithm (Metropolis *et al*. 1953).

$$T_n = \left(\frac{T_1}{T_0} \right)^n T_0 \ , \tag{32}$$

where T_0 is temperature at the beginning (n = 0) and the selected relation $T_1 / T_0 = 0.9$.

Geman & Geman (1984) presented Function (33) for SA methods. This annealing is called the Bolzmann annealing (Ingber 1989).

$$T(n) = \frac{T_0}{\ln(n)} \ , \tag{33}$$

where T is the temperature in the iteration loop n and T_0 is the temperature at the beginning of the optimization process.

In the FSA method, T is lowered according to a specified cooling schedule called the Cauchy annealing (Ingber 1989, Sen & Stoffa 1995).

$$T(n) = \frac{T_0}{n} \ , \tag{34}$$

The difference between these two annealing algorithms (33, 34) in a cooling schedule is clear. The Cauchy method is faster but in practical simulations the rank order of algorithms is not necessarily solved by these kinds of single factors. At the end,

depending on the problem, a fast cooling schedule may need more samples owing to the requirements of the equilibrium of the a posteriori distributions.

In the VSFR method, the annealing algorithm can be changed during the simulation (Ingber 1989). Annealing changes depend on the size of the model space and on the current number of order of the annealing (annealing-time index). In the MFA method (Peterson & Anderson 1987), the step length in the random walk and the temperature of the model are strongly interconnected. As the simulation progresses, the model is ‘annealed’ through the shortening of the step length (by diminishing parameter change).

4. Application in the present study

In the present study, the random simulation and MC inversion were applied to lithospheric thermal models following the schematic algorithm in fig. 4. At first the uniform random numbers were generated using a pseudeo-random number generator (Press *et al*. 1990). The random numbers were transformed into geothermal parameter values in each model at a time. Geometrically, the model was divided into domains the boundaries of which were kept stationary during the simulations. The generation of each variable value was made independently according to the assumed distributions. New models were not dependent on the previous ones, but the random steps were taken simultaneously and independently in all model blocks. The forward problem was solved by a finite difference code SHEMAT (Clauser & Villinger 1990) and the used model parameters and results were collected to a data base. The data base includes all parameter values of all layers in one-dimensional models and all parameter values of all blocks in two-dimensional models as well as the corresponding boundary conditions. Values of model parameters and solutions were not in discrete form (divided into classes) until the investigation of the distribution histograms.

The realization of the simulation algorithm was made in a rather pragmatic and straightforward way. The first major aim was the uncertainty analysis of typical lithospheric modelling. A new model was always generated from the very beginning using a priori model space, thus guaranteeing the prerequisite connection between the uncertainty of model parameters and the uncertainty of results as well as statistical independence were guaranteed. A modified simple random walk increases computational effort in model generation. The second major aim was inversion where the cooling algorithm was rejected. An approved inversion result was reached by accepting proper models to a posteriori model space in the first simulation process. The used thermal state corresponds to the uncertainty of the measured surface HFD data. Due to the inherent ambiguity of the geothermal inversion problem, the simulated annealing was ineffective while realistic surface HFD value was used. In this process, it is not possible to find a ‘best’ model, but only to map the relative probabilities of the different alternatives (see also Mosegaard & Tarantola (1995), for their discussion on the similar problem).

In papers I and II, a priori model spaces were analysed. Uncertainty in both temperature and HFD solutions naturally increases with increasing variation of model parameters. The standard deviations of model parameter distributions and of calculated temperature and HFD distributions were compared and the sensitivity analysis was performed.

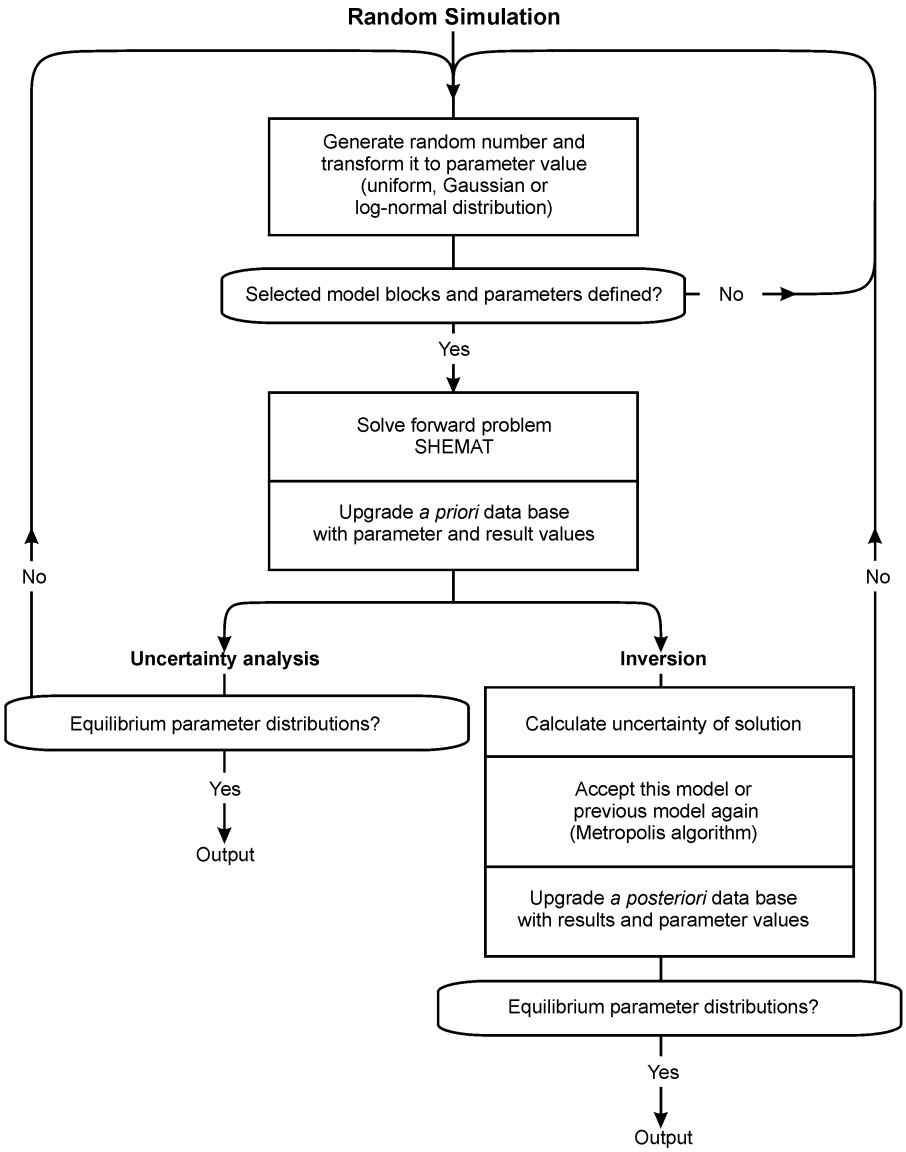

Fig. 4. Application of MC inversion and random simulation techniques in geothermal lithospheric modelling in the present study.

Unlike other normally deviated distributions, heat production was assumed to be log-normally distributed. In paper I, variation of the most important parameters (thermal conductivity and heat production rate, basal boundary conditions, temperature, and HFD) of the conductive lithospheric geothermal model have been studied. In paper II also other parameters (temperature dependence of thermal conductivity and pressure dependence of thermal conductivity) were studied.

When random variation was directed only to rock properties selected boundary conditions were fixed as constant values. Respectively, rock properties were fixed, when the variation was directed to the basal boundary condition only. In combined cases, selected 'constant' basal boundary conditions and parameter values were varied in the simulations, and other basal boundary values were kept constant.

In papers III and IV the samples of the a posteriori model spaces were formed according to the acceptance rules of the Metropolis algorithm. The reached inversion result is the a posteriori model space, consisting of equilibrated distributions of model parameters. Uncertainties of the inversion results are given as standard deviations of inverted temperature and HFD distributions.

In paper IV xenolith-derived temperature data at the mean depth of 208 km (Kukkonen & Peltonen 1999) was added independently to the inverse simulation of the two-dimensional Baltic-SKJ model. Firstly, the inversion was done following the fig. 4 and using the surface HFD data as the fitting object. Secondly, the obtained a posteriori models were mixed into a random order at the same time retaining the connection between the parameters of each model and its results. The existing a posteriori model space was then utilized as a new a priori model space. In the new Metropolis sampling process, the xenolith-derived temperature (with uncertainty) was used as the accepting criterion. This second process was performed without new model generation or new forward calculations. The final a posteriori model space is therefore in agreement with the surface HFD data and xenolith-derived temperatures in the mantle.

5. Publications

The four publications presented in the appendix form an entity where the accuracy of the used thermal models and the application of the MC method in this problem are improved step by step. In the first publication, the MC method used to calculate the accuracy of forward models is presented. In addition to uncertainty analysis, the effects of each most important model parameter on the accuracy of the results of the thermal models were studied (sensitivity analysis). The second work concentrates on accuracy and sensitivity analysis of the modelling results on the temperature and pressure dependencies of the thermal conductivity of rocks. In the third paper, the uncertainty of the thermal model is decreased by applying Metropolis sampling, thus setting acceptance conditions for calculated surface HFD variation. The used inversion method improves both the results and the model parameter distributions. In the fourth publication, the two-dimensional model of the Baltic-SKJ transect is improved by entering xenolith-derived mantle temperature data into the inversion.

5.1. Paper I

Jokinen J & Kukkonen IT (1999a) Random modelling of the lithospheric thermal regime: forward simulations applied in uncertainty analysis. In: Clauser C, Lewis T & Rybach L (eds.) Thermal regimes in the continental and oceanic lithosphere: selected papers of the symposium “Heat flow, seismic structure and seismicity in active tectonic regimes” and the workshop “Thermal regimes in the continental and oceanic lithosphere”, held during the 29th General Assembly of the International Association of Seismology and Physics of the Earth’s Interior (IASPEI), Thessaloniki, Greece, August 18–28, 1997. Tectonophysics 306 (3-4): 277–292.

Random modelling technique was applied in uncertainty analysis of forward geothermal modelling of the lithospheric thermal regime. Results are presented for estimating the effects of uncertainties in thermal conductivity, heat production rate, model basal temperature, and basal heat flow density on calculated lithospheric temperature and

HFD. Two models were analysed, first a 4-layer synthetic model representative of typical shield conditions with thick crust and lithosphere, and secondly a 2-dimensional case history from the Fennoscandian (Baltic) Shield.

Thermal conductivity (normally distributed) and heat production (log-normally distributed) as well as temperature or HFD (normally distributed, used as the lower boundary condition in the mantle) were randomly varied in the simulation. Calculations based on 1500 independent cases of the layered model indicate, for instance, that a standard deviation (STD) of 50 K in calculated Moho temperature results in uncertainties either in thermal conductivity of about 0.5 W m^{-1} K^{-1}, in heat production rate of 0.2 $\log_{10}$ A (A in μW m^{-3}), 115 K in basal temperature or 1.7 mW m^{-2} in basal HFD. Again, the same values result in the uncertainty of about 2 mW m^{-2} in calculated Moho HFD and 10 mW m^{-2} in calculated surface HFD.

If conductivity and heat production rate are varied simultaneously, the resulting uncertainty in calculated Moho temperature increases to about 70 K. Adding also basal temperature variation increases the Moho temperature variation to about 85 K. Results calculated using the 2-dimensional Baltic Shield transect indicate analogously that uncertainty of temperature at the depth of 50 km (approximately at the Moho) is 35–60 K (using temperature as the lower boundary condition) and 50–85 K (using HFD as lower boundary condition). The corresponding variations in surface HFD are 6–15 mW m^{-2}.

5.2. Paper II

Kukkonen IT, Jokinen J & Seipold U (1999) Temperature and pressure dependencies of thermal transport properties of rocks: Implications for uncertainties in thermal lithosphere models and new laboratory measurements of high-grade rocks in the Central Fennoscandian Shield. Surveys in Geophysics 20: 33–59.

Measurements on thermal conductivity and on diffusivity as functions of temperature and pressure are presented for Archaean and Proterozoic mafic high-grade rocks metamorphosed in middle and lower crustal pressures, and situated in the central Fennoscandian Shield. Decrease of 12–20 % in conductivity and 40–55 % in diffusivity was recorded between room temperature and 1150 K, which may be considered typical of phonon conductivity. Radiative heat transfer effects were not detected in these samples. Pressure dependencies (up to 1000 MPa) of the samples are weak if compared to crystalline rocks in general, but relatively typical of mafic rocks.

The temperature and pressure dependencies of thermal transport properties (data from literature and the present study) were applied in an uncertainty analysis of lithospheric conductive thermal modellings with random (MC) simulations using a 4-layer model representative of the shield lithosphere. Model parameters were varied according to predetermined probability functions and standard deviations were calculated for lithospheric temperature and HFD after 1500 independent simulations. The results suggest that the variations (uncertainties) in calculated temperature and HFD values due to variations in the temperature and pressure dependencies of conductivity are minor in comparison to the effect produced by typical variations in the room temperature value of conductivity, heat production rate or lower boundary condition values.

5.3. Paper III

Jokinen J & Kukkonen IT (1999b) Inverse simulation of the lithospheric thermal regime using the Monte Carlo method. In: Clauser C, Lewis T & Rybach L (eds.) Thermal regimes in the continental and oceanic lithosphere: selected papers of the symposium "Heat flow, seismic structure and seismicity in active tectonic regimes" and the workshop "Thermal regimes in the continental and oceanic lithosphere", held during the 29th General Assembly of the International Association of Seismology and Physics of the Earth's Interior (IASPEI), Thessaloniki, Greece, August 18–28, 1997. Tectonophysics 306 (3-4): 293–310.

The MC inversion method was applied to geothermal lithospheric models of conductive heat transfer in steady-state conditions. A priori models were generated from probability distributions assigned to thermal conductivity and heat production rate of the models. Corresponding temperature and HFD values were calculated numerically, and the modification of the a priori distributions into samples of the a posteriori distributions was carried out using the Metropolis algorithm as the acceptance rule and surface HFD values as a fitting object. Two models were analysed, first a 1-dimensional layered earth model with three crustal and one upper mantle layer, and secondly, a 2-dimensional lithospheric model in Fennoscandian Shield. The thermal conductivity and heat production rate were either (1) evenly or (2) normally and log-normally distributed in the models. In both cases the results were generally similar in the sense that the same kinds of changes were suggested by the inversion algorithm for conductivity, heat production rate, temperature, and HFD, although the changes were not identical in details.

The result indicates that the inversion tool is robust and able to reach solutions from relatively loosely constrained a priori parameter estimates. However, the general ambiguity of the geothermal inversion problem influences the results considerably. The MC inversion can be used for analysing the problem with the aid of the a posteriori distributions of different parameters. Improvement of results, i.e. shifting of mean values and narrowing of distributions were observed in many domains of the models. Deterioration of the parameter estimates was not recorded.

5.4. Paper IV

Jokinen J & Kukkonen IT (2000) Inverse Monte Carlo simulation of the lithospheric thermal regime in the Fennoscandian Shield using xenolith-derived mantle temperatures. Journal of Geodynamics 29: 71 – 85.

MC inversion was applied in 2-dimensional conductive steady-state thermal simulation of a 600 km long lithosphere transect in the Fennoscandian Shield. The thermal regime in the mantle was constrained with thermobarometric data derived from kimberlite-hosted mantle xenoliths in eastern Finland, which suggest an average temperature of 1250 ± 50 °C (1523 ± 50 K) at 208 km, but no partial melting down to at least 240 km. A priori models were generated from probability distributions assigned to thermal conductivity and heat production rate values, as well as to the mantle HFD used as the lower boundary condition in the simulations. The forward problem was solved with

the finite difference code, and the modifications of the a priori distributions into a posteriori distributions were carried out using the Metropolis algorithm. The two-stage inversion, firstly using the measured surface HFD values as a fitting object, and secondly, re-sampling the obtained a posteriori models but using xenolith-derived mantle temperature data as a fitting object, results in a considerable improvement in the resolution and average values of temperature and HFD in the model. The improvements can be seen in the model results to a distance of about 400 km from the xenolith area. The obtained results support a scheme that the mantle HFD is low in the thickest lithosphere area of Fennoscandian Shield and about 10 ± 1 mW m^{-2} at about 200 km, and 13 ± 1 mW m^{-2} in the uppermost subcrustal mantle. The inversion results suggest, that there is no partial melt-bearing asthenosphere under the transect at depths shallower than at least 250 km. The seismic lithosphere-asthenosphere boundary is at depths of 110–170 km on the transect and corresponds to a temperature of about 1100 °C (1373 K) in the model. This transition can be related to a zone of rheological weakening but not to the onset of melting. The mantle temperature and HFD value in the Eastern Finland kimberlite province are in agreement with models where small-scale convection (solid state creep) transports heat to the base of the lithosphere at the depth of about 250 km.

6. Discussion and conclusions

The major achievements of the present dissertation are the following: (1) uncertainty analysis of typical lithospheric thermal models, (2) assessment of the uncertainties of function of the individual uncertainties of input thermal parameters and boundary conditions, and (3) application of MC inversion methods in geothermal modelling.

The results of the uncertainty analysis can be generalized to apply to Precambrian shields on a large scale. With caution, they can also be used for the Phanerozoic stabilized continental crust where the crustal and lithosphere thicknesses are comparable to the present models. And certainly, the qualitative conclusions on the relative importance of different uncertainties of simulation results are valid in other continental areas as well.

The uncertainty analysis and inversions suggest that e.g. the Moho temperature (a typical variable presented in geothermal maps) can be obtained with an uncertainty at c. 60–90 K, when the modelling is based on using surface HFD data as a fitting object. This value can be decreased if there are other data on deep temperatures, independent of the measured HFD values, as was shown by the 2-D inversion utilizing xenolith-temperatures.

In addition to utilizing xenolith-temperatures another method may be provided e.g. by the use of data on the temperature dependence of seismic P-wave velocity obtained from tomographic inversion studies on upper mantle (Furlong *et al*. 1995) or possibly by the temperature dependence of conductivity in mantle in magnetotelluric studies (Korja 1990). Reciprocally, geothermal models with uncertainty analyses complete research work where model parameters are temperature dependent. Facilities to combine different geosciences have been improved during frame projects such as the EUROPROBE (Gee & Zeyen 1996) and SVEKALAPKO (Hjelt 1997) projects. Results from the Fennoscandian Shield have recently been published within the GGT / SVEKA project (Korsman *et al*. 1999).

The most important parameters contributing to total modelling uncertainty are the lower boundary condition, thermal conductivity, and the heat production rate. Pressure and temperature dependencies of thermal conductivity are less important as long as the general levels of thermal conductivity are correctly chosen in the model.

Generally, any model is only as reliable as its input data, and this applies particularly to thermal properties and their pressure and temperature dependencies. In the lithosphere, temperature and pressure may range up to about 1800 K and 7000 MPa, respectively. The laboratory measurements of thermal conductivity in this study correspond to a maximum depth value of about 100 km for temperature dependent measurements (up to 1150 K) and about 34 km for pressure dependent measurements (up to 1000 MPa). There is still lack of knowledge, comprehensive data sets on lower crustal and upper mantle materials that could be used in simulated in situ conditions involving simultaneous control of both pressure and temperature. Extrapolation of the linear pressure dependence of thermal conductivity to pressures prevailing in the lower lithosphere suggests that the thermal decrease of phonon conductivity may be partly or completely compensated by the pressure-induced increase in the conductivity of upper mantle rocks at depths exceeding 100 km. The problem is further complicated by the radiative heat transfer effects.

MC inversion was noted to be a practical tool in geothermal modelling, capable of improving the models, i.e. of shifting the mode values of distributions and narrowing them. However, the inherent ambiguity of thermal models cannot be avoided, even if the measured data were perfect. The demonstration of non-uniqueness (Fig. 4 in paper III) indicated that it is relatively easy to find an acceptable model using typical forward simulation (try-and-error estimation of model parameters) but the representativeness of such results is much more difficult to judge.

This implies that thermal lithosphere thickness estimation in shields, based on the downward continuation of a geotherm (temperature-depth curve) until it intersects a solidus curve or a mantle adiabat, may include considerable uncertainties. If the temperature gradient in the mantle is of the order of 4–5 K km^{-1} and the uncertainty of temperature calculation may exceed 200 K at the depth of 150 km (Fig. 8 in paper III), the thermal lithosphere thickness estimate is obtained with an uncertainty of about 50 km. Surely it is not surprising that mantle melting curves (Pollack & Chapman 1977) and geotherm families (Pollack *et al*. 1993), which are generally used as tools in continental and lithospheric studies, have uncertainties. However, now these uncertainties have been mapped as well.

The present applications of random modelling and MC inversion were realized in a stationary way, i.e. the boundaries between individual domains were kept constant in all models and spatial autocorrelation of thermal conductivity or heat production rate was not included either. It would be possible to modify the model generation scheme accordingly, and to accomplish it using e.g. the continuum approach (Niemi 1994). However, the major complication is the lack of real autocorrelation data. The data on the Fennoscandian Shield are too sparse for a reasonable variogram analysis of thermal conductivity. Radiogenic heat production has been surveyed extensively in Finland (Kukkonen 1989a,b, 1993, Jõeleht & Kukkonen 1998) using either glacial till or outcrop samples, but so far, no variogram study has been presented. However, the autocorrelation analysis is an important aspect which should be developed further in future studies. As for thermal conductivity, some associated information could be obtained from other studies on extensively surveyed petrophysical properties of rocks. However, the correlation between density and thermal conductivity was generally poor in the Finnish data set (Kukkonen & Peltoniemi 1998).

Calculated uncertainties do not weaken previous geothermal models. It has been concluded that thermal parameters vary in the earth and average values of model units cannot be defined accurately for the subsurface. The normal variation of the physical properties of geological and lithological units causes uncertainty in the models. The random simulation method is proved to be a practical tool for improving geothermal models. This work clearly demonstrates how accurate geothermal investigations into the thick continental crust have been carried out effectively and also how these can be still improved.

7. References

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