POSIVA 99-01

Measurement of thermal conductivity and diffusivity in situ: Literature survey and theoretical modelling of measurements

Ilmo Kukkonen
Ilkka Suppala
Geological Survey of Finland

30 - 17

January 1999

POSIVA OY
Mikonkatu 15 A, FIN-00100 HELSINKI, FINLAND
Phone (09) 2280 30 (nat.), (+358-9-) 2280 30 (int.)
Fax (09) 2280 3719 (nat.), (+358-9-) 2280 3719 (int.)

ISBN 951-652-056-1
ISSN 1239-3096

Posiva-raportti - Posiva Report

Posiva Oy
Mikonkatu 15 A, FIN-00100 HELSINKI, FINLAND
Puh. (09) 2280 30 - Int. Tel. +358 9 2280 30

Raportin tunnus - Report code
POSIVA 99-01

Julkaisuaika - Date
January 1999

Tekijä(t) - Author(s)

Ilmo Kukkonen
Ilkka Suppala
Geological Survey of Finland

Toimeksiantaja(t) - Commissioned by

Posiva Oy

Nimeke - Title

MEASUREMENT OF THERMAL CONDUCTIVITY AND DIFFUSIVITY IN SITU: LITERATURE SURVEY AND THEORETICAL MODELLING OF MEASUREMENTS

Tiivistelmä - Abstract

In situ measurements of thermal conductivity and diffusivity of bedrock were investigated with the aid of a literature survey and theoretical simulations of a measurement system. According to the surveyed literature, in situ methods can be divided into 'active' drill hole methods, and 'passive' indirect methods utilizing other drill hole measurements together with cutting samples and petrophysical relationships. The most common active drill hole method is a cylindrical heat producing probe whose temperature is registered as a function of time. The temperature response can be calculated and interpreted with the aid of analytical solutions of the cylindrical heat conduction equation, particularly the solution for an infinite perfectly conducting cylindrical probe in a homogeneous medium, and the solution for a line source of heat in a medium.

Using both forward and inverse modellings, a theoretical measurement system was analysed with an aim at finding the basic parameters for construction of a practical measurement system. The results indicate that thermal conductivity can be relatively well estimated with borehole measurements, whereas thermal diffusivity is much more sensitive to various disturbing factors, such as thermal contact resistance and variations in probe parameters. In addition, the three-dimensional conduction effects were investigated to find out the magnitude of axial 'leak' of heat in long-duration experiments.

The radius of influence of a drill hole measurement is mainly dependent on the duration of the experiment. Assuming typical conductivity and diffusivity values of crystalline rocks, the measurement yields information within less than a metre from the drill hole, when the experiment lasts about 24 hours.

We propose the following factors to be taken as basic parameters in the construction of a practical measurement system: the probe length 1.5-2 m, heating power 5-20 W m^{-1}, temperature recording with 5-7 sensors placed along the probe, and duration of a measurement up to 100 000 s (about 27.8 hours). Assuming these parameters, the interpretation of measurements can be done using the readily available inversion modelling methods based on the solution for the infinitely long cylinder. Experiments with a longer duration can be interpreted using numerical solutions for finite cylinders.

Avainsanat - Keywords
thermal conductivity, thermal diffusivity, measurement methods, in situ, modelling, crystalline rocks, nuclear waste

ISBN ISBN 951-652-056-1	ISSN ISSN 1239-3096
Sivumäärä - Number of pages 69	Kieli - Language English

Posiva-raportti - Posiva Report

Posiva Oy
Mikonkatu 15 A, FIN-00100 HELSINKI, FINLAND
Puh. (09) 2280 30 - Int. Tel. +358 9 2280 30

Raportin tunnus - Report code
POSIVA 99-01

Julkaisuaika - Date
Tammikuu 1999

Tekijä(t) - Author(s)	Toimeksiantaja(t) - Commissioned by
Ilmo Kukkonen Ilkka Suppala Geologian tutkimuskeskus	Posiva Oy

Nimeke - Title

LÄMMÖNJOHTAVUUDEN JA TERMISEN DIFFUSIVITEETIN IN SITU -MITTAUS: KIRJALLISUUSSELVITYS JA MITTAUSTEN TEOREETTINEN MALLINTAMINEN

Tiivistelmä - Abstract

Tässä raportissa on selvitetty kallion termisten ominaisuuksien (lämmönjohtavuus ja terminen diffusiviteetti) määrittämistä *in situ* -mittauksin. Kirjallisuuden perusteella voidaan *in situ* -menetelmät jakaa aktiivisiin reikämittausmenetelmiin ja passiivisiin reikägeofysikaalisia mittauksia, jauhenäytteitä ja petrofysikaalisia relaatioita hyödyntäviin epäsuoriin menetelmiin. Tavallisin kirjallisuudessa raportoitu menetelmä on kairanreikään asennettava hyvinjohtava sylinterinmuotoinen lämpölähde, jonka lämpötilaa mitataan ajan funktiona. Lämpötilavaste voidaan laskea analyyttisistä lämmönjohtavuuden differentiaaliyhtälön ratkaisuista, joita tunnetaan äärettömän pitkälle sylinterimuotoiselle johteelle ja viivamaiselle lämpölähteelle.

Sekä suorien että käänteismallitusten avulla tutkittiin em. ratkaisujen avulla teoreettisen mittausjärjestelmän ominaisuuksia tavoitteena löytää suunnitteluparametrit toteuttamiskelpoiselle reikämittauslaitteelle. Tehdyt simuloinnit osoittavat, että lämmönjohtavuus on varsin hyvin estimoitavissa reikämittauksen avulla, mutta diffusiviteetti on huomattavasti herkempi anturin ja reiän seinän välisen kontaktiresistanssin ja anturiparametrien vaihteluille.

Kairanreiässä tehtävän *in situ* -mittauksen vaikutussäde on riippuvainen lähinnä lämmityksen ja mittauksen kestosta. Tyypillisillä kivien johtavuus- ja diffusiviteettiarvoilla yksireikämittaus tuo informaatiota kiven ominaisuuksista alle metrin etäisyydeltä, kun kokeen kestoaika on noin 1 vrk.

Käytännön mittausjärjestelmän suunnittelun pohjaksi esitetään seuraavia lähtöarvoja: Anturin pituus 1.5-2 m, lämmönsyöttöteho 5-20 W m^{-1}, lämpötilan mittaus 5-7:llä pitkin anturia sijoitetulla lämpötilasensorilla, ja mittauksen kestoaika 100 000 sekuntiin (noin 27.8 h) asti. Tulkinta voidaan näillä lähtöarvoilla tehdä käyttäen jo kehitettyjä käänteisen tulkinnan menetelmiä, jotka perustuvat äärettömän pitkän sylinterin lämpötilavasteeseen. Pitempiaikaiset mittaukset voidaan tulkita äärellisen pituisen sylinterilähteen numeerisen ratkaisun avulla.

Avainsanat - Keywords
lämmönjohtavuus, terminen diffusiviteetti, mittausmenetelmät, in situ, mallintaminen, kiteiset kivilajit, ydinjäte

ISBN	ISSN
ISBN 951-652-056-1	ISSN 1239-3096
Sivumäärä - Number of pages	Kieli - Language
69	Englanti

Preface

This study was carried out at the Geological Survey of Finland on a contract for Posiva Oy. Ilmo Kukkonen was responsible for coordination of the project, the literature survey, report compilation and Ilkka Suppala for the theoretical modellings. The work has been supervised by Aimo Hautojärvi at Posiva and Erik Johansson at Saanio & Riekkola Consulting Engineers.

TABLE OF CONTENTS

1 INTRODUCTION

The present study is related to the investigations of Posiva Oy for disposing spent nuclear fuel in the Finnish bedrock at depths of about 300-700 m. Investigations are currently underway at four investigation sites.

Due to the radiogenic heat production of the spent fuel, the thermal regime of the bedrock in the repository and its surroundings is expected to change (Raiko, 1996). Thermal properties, particularly thermal conductivity and diffusivity are essential material parameters of the bedrock controlling the heat transfer and temperature increase in the vicinity of the repository. Previous studies on the thermal properties of rocks at the Romuvaara, Olkiluoto, Kivetty and Hästholmen sites have been reported by Kukkonen and Lindberg (1995, 1998). In these studies drill core samples were investigated using laboratory measurements as well as indirect estimation methods based on mineral composition of the samples.

Drill core samples are representative for thermal properties in a small specimen scale, but there is a need to enlarge the scale of investigations into metres and beyond. This implies that measurements must be carried out *in situ* in boreholes.

The aim of the present study is to summarize literature data on thermal property measurements *in situ* as reported for various purposes in geothermal, waste disposal and other projects. Further, the results are used for a preliminary characterization of a possible measurement system to be used in the Finnish spent nuclear fuel programme. We present a forward and inverse modelling analysis of a measurement system for single holes, and present a number of suggestions to be taken into account in the practical probe construction.

2 FACTORS CONTRIBUTING TO THE THERMAL TRANSPORT PROPERTIES OF ROCKS

The thermal transport properties of rocks are thermal conductivity and diffusivity. They are related to the specific heat and density according the the following relation

$$s = \lambda/(\rho c) \tag{1}$$

where s is thermal diffusivity ($m^2\ s^{-1}$), λ is thermal conductivity ($W\ m^{-1}\ K^{-1}$), c is specific heat ($J\ kg^{-1}\ K^{-1}$) and ρ is density ($kg\ m^{-3}$).

Thermal conductivity and diffusivity of rocks are primarily controlled by the mineral composition, texture, porosity, and pore filling fluids. The most typical rock forming minerals have thermal conductivities in the range of 1.7 to 11.3 $W\ m^{-1}\ K^{-1}$, but typically crystalline rocks have conductivites in the range of 2-5 $W\ m^{-1}\ K^{-1}$. The diffusivities of crystalline rocks are in the range of $0.5\text{-}2.0 \cdot 10^{-6}\ m^2\ s^{-1}$.

The factors influencing on conductivity have been shortly discussed by Kukkonen and Lindberg (1995), and in greater detail by, e.g. Clauser and Huenges (1995).

In addition, the prevailing temperature and pressure also influence the values of conductivity and diffusivity. Temperature increasing from room temperature decreases thermal conductivity and diffusivity by about 40-60 % until a temperature of about 800-1000°C is reached. Above this value thermal conductivity often shows an increase with temperature. This is due to the gradually increasing contribution of radiative heat transfer.

The scale of sampling may also have an effect on the thermal transport properties. In the laboratory sample scale the thermal conductivity measurements may show a scatter of results if the characteristic dimension of the mineral texture of rock approaches the sample size. This kind of features were observed in the previous investigations by Kukkonen and Lindberg (1995, 1998), where the coarse granites and granodiorites with porphyroblasts of several cm in diameter were cut in the samples. Increasing the scale from laboratory sample scale to outcrop (5-50 m) or formation scale (100-1000 m and beyond) brings the effect of different rock types with contrasting thermal conductivities producing structural anisotropy and channelling of heat, which results in local anomalies in heat flow density as well as bending of the isotherms. The average thermal conductivity may not be very different if determined from either large or small samples, but the variation of values can be expected to decrease with increasing scale of investigation. Further, in the scale of a formation (or a repository site), the fluid-filled fracture zones which cannot be sampled for laboratory measurements of thermal properties, may also create differences in conductivities *in situ* in comparison to average values derived from laboratory measurements.

3 FINAL DISPOSAL OF SPENT FUEL IN BEDROCK: THE DEMANDS FOR DATA ANALYSIS OF THE THERMAL TRANSPORT PROPERTIES OF BEDROCK

The present plans of the final disposal of spent nuclear fuel in the Finnish bedrock are based on the following concept. A system of tunnels is excavated at the depth of about 300-700 m, and the fuel elements are disposed in steel-copper canisters in vertical, about 10 m long boreholes stuffed with bentonite as buffer material (Fig. 1). The heat generation of the canisters depends on the time allowed for the fuel elements to cool after use in a nuclear reactor. By mixing elements with different cooling times before disposal it is possible to have approximately constant heat production of the canisters during the first 25 years after disposal (Raiko, 1996). According to numerical simulations, the maximum temperatures at the canister surfaces can be expected to appear during this time. Due to the properties of the bentonite buffer, the temperature at the canister-bentonite interface should not exceed 100°C for a long period of time. The maximum temperature can be controlled by the number of fuel elements in a canister, its length/diameter ratio as well as the distance between canister holes, and it also depends on the thermal properties of the surrounding bedrock and the bentonite buffer. High thermal conductivity is preferred as it insures the efficient removal of heat from the bentonite layer.

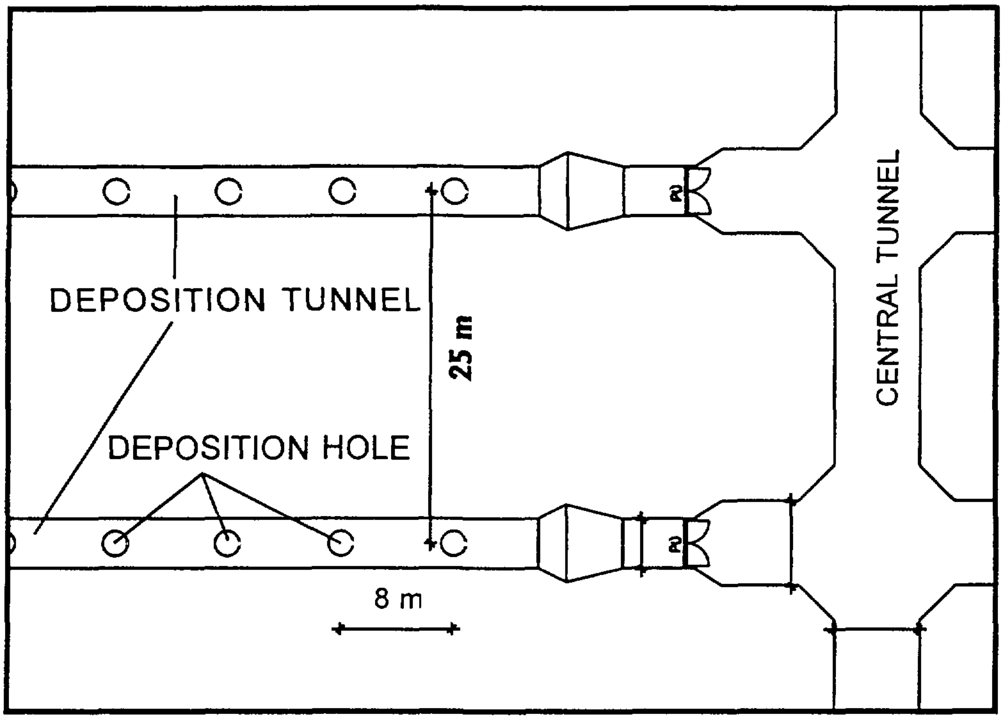

Figure 1. *Schematic layout of deposition tunnels and holes.*

The simulations of the thermal conditions in the repository by Raiko (1996), and calculated for a nominal thermal conductivity of 3.0 $Wm^{-1} K^{-1}$ suggest that 10% decrease in the thermal conductivity increases the maximum temperature at the bentonite-canister interface by about 4 % from the nominal value of 81 °C. The tunnels are planned to be placed at distances of about 25 m from each other and the canister holes at distances of about 6-8 m. A 10 % decrease in these parameters produces about 4-6 % increase in the temperature at the canister-bentonite interface.

From the repository concept it can be seen, that the ideal scale of investigation of an *in situ* measurement should preferably be in the range of 6-25 m. However, the conduction of heat will put its own constraints on the measurement system, and considerable times are needed if such a distance is to be controlled by borehole measurements. This can be attributed to the slow propagation of thermal signals in rock. This problem is further discussed in later sections of this report.

The previous modellings (Raiko, 1996) were done using thermal conductivity values measured in laboratory and an estimated value of specific heat as well as rock density. The time dependent solutions were then calculated using a diffusivity value calculated from eq. 1. However, it would be practical if the thermal diffusivity could be measured not only in laboratory (e.g. Kukkonen and Lindberg, 1998) but also *in situ*. Therefore, a useful *in situ* measuring system should be capable of measuring both conductivity and diffusivity *in situ*.

4 DETERMINATION OF THERMAL TRANSPORT PROPERTIES OF ROCKS IN THE LABORATORY SAMPLE SCALE

There are several methods for measuring thermal conductivity and diffusivity in the laboratory. The methods can basically be divided into steady-state and transient methods. A good summary of the most often used techniques is given by Beck (1988).

The most common steady-state method of measuring thermal conductivity in the laboratory is the divided-bar method (Fig. 2). In this method, the sample is placed in the middle of a bar (or column) consisting of alternating sections of known conductivity standards (typically quartz or glass) and high conductivity material (e.g. copper) in which temperature sensors are placed. The upper and lower ends of the bar are kept at different constant temperatures, and thus a flux of heat through the bar is created. By measuring temperature differences across the sample and the conductivity references after reaching stationary conditions, the thermal conductivity of the sample can be calculated. The method is very reliable, but demands careful preparation of the samples.

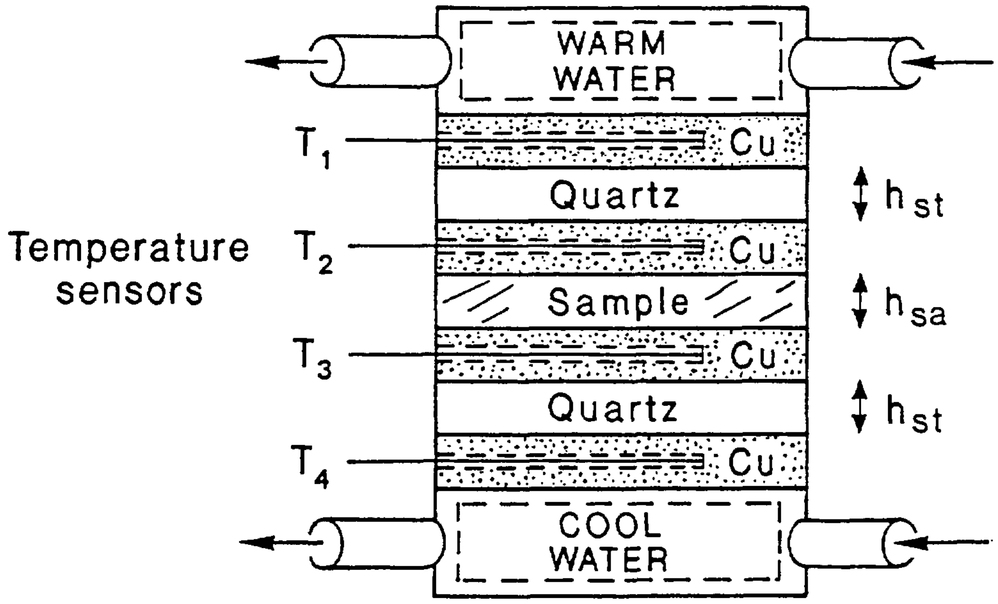

Figure 2. *The divided-bar method for thermal conductivity measurements (Kukkonen and Lindberg, 1995).*

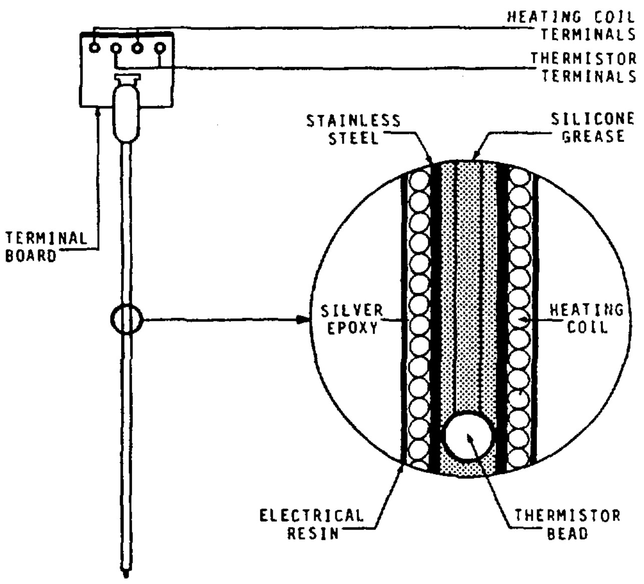

Figure 3. *Typical needle probe arrangement (Beck, 1988). Probe diameter is usually 1-3 mm.*

The most typical transient method is the transient linear heat source method, often called 'needle probe method' (Fig. 3). This is based on the transient response of a long line source of heat which is generating heat at a constant rate. (The conduction of heat in such a geometry is discussed in detail in chapter 6.) After a while, the temperature increase of the probe becomes linear with logarithm of time, and the thermal conductivity estimate can be calculated from the slope of the line. Thermal diffusivity can also be determined with this method by using the response for small times, or the intercept of the linear response with the time axis. The method has been extensively used for studies of soft sediments and sedimentary rocks, as well as chip samples mixed with water. The contact resistance between the probe and the medium may be problematic.

Diffusivity can also be determined by the Ångström method. A periodically variable temperature signal is input in the sample on one surface and the time dependent temperature changes are measured at two distances from the source. A geothermal application is provided by Drury et al. (1984).

The thermal properties can also be determined indirectly in the laboratory from other petrophysical properties and the mineral composition of the samples. The latter alternative was used by Kukkonen and Lindberg (1995, 1998) for estimating the thermal properties of the samples from the investigation sites in the Finnish nuclear waste management programme. In such a method one needs to know the thermal properties of the rock forming minerals, the values of which are readily available in the literature (e.g., Birch and Clark, 1940; Horai, 1971; Cermak and Rybach, 1982; Clauser and Huenges, 1995; Popov et al., 1987). However, the texture, grain size and anisotropy of the rocks have a controlling role in the exact values. Usually estimates can be constrained by the arithmetic, geometric and harmonic mean estimators, or combinations of these, such as the Hansen-Strikhman estimators (Pribnow and Sass, 1995).

The estimation of the thermal properties with the aid of relationships between them and other petrophysical parameters can also be used, and their existence can be also theoretically argumented for in certain cases, but generally, a study of a Finnish data set (2500 Precambrian rock samples) suggested that the many different factors involved make the relationships very scattered (Kukkonen and Peltoniemi, 1998). However, if the lithological types of rocks are not very variable, the relationships may be less scattered (Kukkonen and Lindberg, 1998; Pribnow and Sass, 1995; Brigaud et al., 1990, 1989; Williams et al., 1988).

5 DETERMINATION OF THERMAL TRANSPORT PROPERTIES OF ROCKS IN SITU

5.1 Introduction

Thermal conductivity has been determined *in situ* for a considerable number of applications. Most of them are related to studies of the terrestrial heat flow density for purposes of geophysical research (Beck et al., 1971; Sass et al., 1981; Jolivet and Vasseur, 1982; Kristiansen, 1982), super-deep drill hole studies (Burkhardt et al., 1990, 1995), geothermal energy exploration (Behrens et al. 1980; Mussmann and Kessels, 1980), ground heat exchanger studies, nuclear waste studies as well as other studies related to different kinds of industrial waste materials with thermal relevance or heat generation (Hodgkinson and Bourke, 1978; Cook and Witherspoon, 1978; Hocking et al., 1981; Kopietz and Jung, 1978; Rotfuchs, 1978; Chan and Jeffrey, 1983, Tan and Ritchie, 1997).

In situ measurements have many advantages in comparison to laboratory measurements. The most important thing is the ability to measure the thermal properties in place, and in the prevailing ambient conditions. Thus the effect of fluids in the pores and fractures of the rock are automatically included in the investigation. Further, the scale of measurement can be made much bigger than in the laboratory, and it helps essentially in estimating thermal conductivity of heterogeneous rocks, but in practice the scale of investigation cannot be increased infinitely, as this is limited by the slow conduction of heat in rocks. A further advantage of *in situ* measurements is the fact that core drilling is not necessary for determining the thermal transport properties, which helps in making investigations more cost-effective.

Thermal anisotropy of rock is easily measured in the laboratory with proper sample preparation, but in measurements *in situ* this is limited, sometimes impossible. For instance, the typical transient line or cylindrical source methods discussed below in many applications as well as in our simulations, yield thermal conductivity values which are representative only in the plane perpendicular to the source (borehole). This is a problem in geothermal studies where the temperature gradient measured in a borehole should be multiplied by the vertical component of thermal conductivity to obtain the value of geothermal heat flow density. If the formation has significant thermal anisotropy, the results interpreted with a transient cylindrical or line source solution are not representative. An early application of numerical modelling of a cylindrical probe conduction in an anisotropic medium was presented by Wright and Garland (1968).

Several techniques have been applied in measurements of thermal parameters *in situ*, such as 'passive' methods based on either temperature gradients in a borehole as indicators of lithologic (conductivity) variation (Conaway and Beck, 1977), annual temperature wave in the uppermost 15-30 m of bedrock for diffusivity determination (Parasnis, 1974; Tan and Ritchie, 1997), or direct measurement of geothermal heat flow density and simultaneous temperature gradient in a drill hole which can be used for *in situ* conductivity estimation (Oelsner and Rösler, 1981; Jolivet and Vasseur, 1982). Various active methods using either cylindrical, line or spherical sources for generating either a continuos heating signal or a heat pulse in the investigated medium have been developed for measurements in boreholes or soft sediments for terrestrial, marine and lunar studies (e.g. Beck et al., 1971; Sass et al., 1981; Mussman and Kessels, 1980; Langseth et al., 1972; Davis, 1988). By far the most popular methods for measurements in a borehole or equivalent opening in the target medium are based on these methods.

The basic theory of heat conduction in a cylindrically symmetric geometry is developed by Carslaw and Jaeger (1959), Jaeger (1955, 1958,1959) and Blackwell (1953, 1954, 1956). They discussed analytical solutions for an infinitely long conductive cylinder which produces heat dissipating to the surrounding medium. When the cylinder is placed in an infinite medium and it generates heat at constant power, the temperature of the cylinder increases with time in a characteristic way (Fig. 4). After an initial phase the temperature remains increasing at a constant rate. Theoretically, the slope of this equilibrium line is inversely proportional to thermal conductivity and the intercept of the linear part on the time axis can be used for determining thermal diffusivity. There are numerous applications of thermal conductivity measurements based on this solution, both in laboratory as well as *in situ* scales.

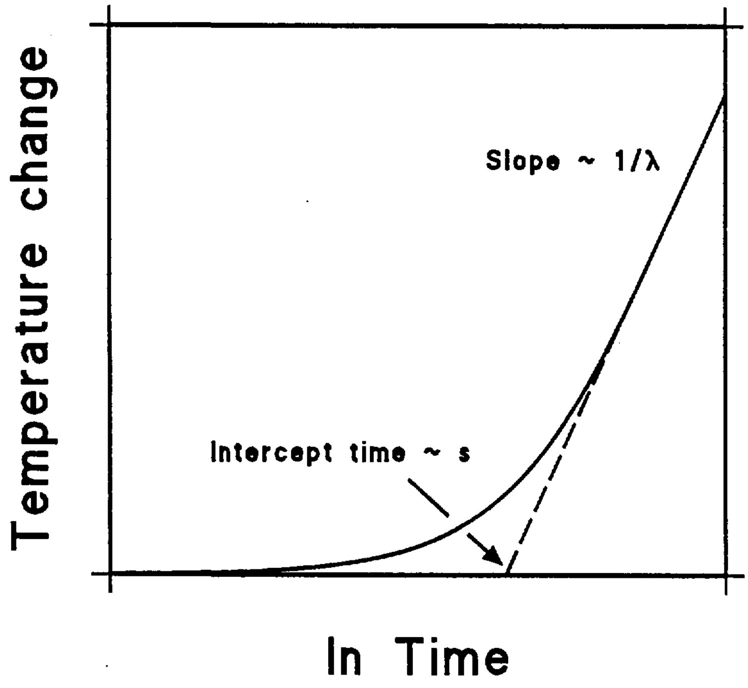

Figure 4. *Schematic temperature response of a cylindrical heat source in a homogeneous medium.*

The mathematics of this basic solution is discussed in detail in the next chapter, and therefore these issues are discussed only shortly here. The solution of the equation of heat conduction in a cylindrical symmetric geometry contains Bessel functions of the first and second kinds. Numerical values of the solution can be obtained with series approximations for certain special cases, such as very short and very long measurement times. They have been widely used in several applications of the method, but also numerical solutions of the heat conduction equation have been used.

The most important factors involved in the transient cylindrical source solutions and the thermal response of a measurement system are (1) the rock thermal conductivity, (2) diffusivity (or volumetric heat capacity and density), and (3) the contact resistance between the probe and borehole wall. In addition, also the length of the probe in relation to the borehole diameter is an important factor affecting the three-dimensional effects of heat conduction in practice. The ends of the probe 'leak' heat in the axial direction and an assumption of the infinitely long cylinder may not be valid for long measurement times.

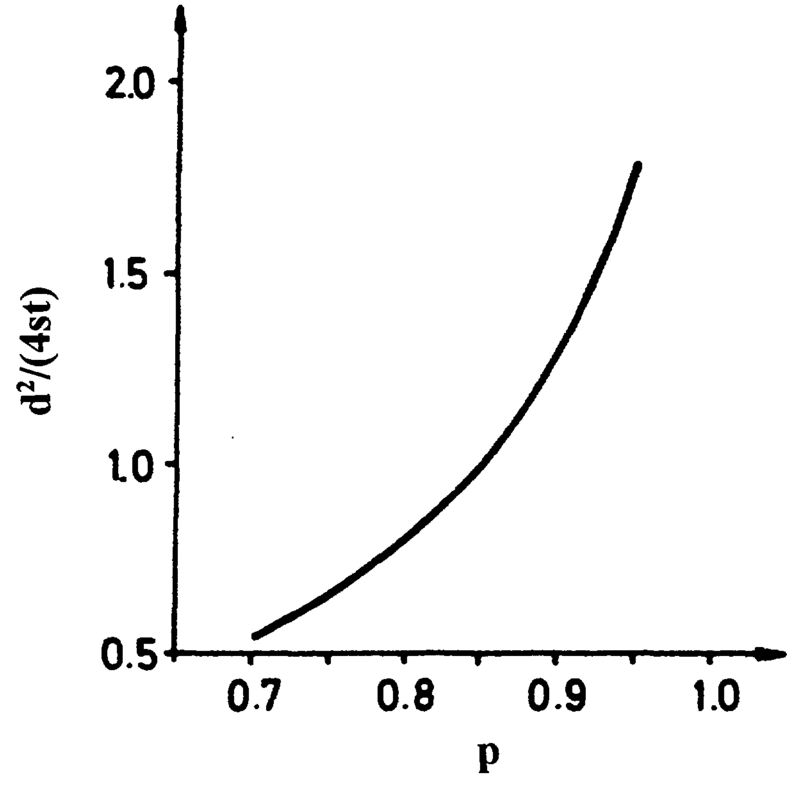

Figure 5. *Non-dimensional distance of heat conducted from a continuous line source as a function of the relative fraction of total energy conducted to the medium and within distance d. The graph can be used for estimating the radius of influence of a transient measurement (adapted from Kristiansen, 1982)*

The problem of the representative volume of a measurement is dependent on the duration of measurement. Kristiansen (1982) investigated this problem, and presented a relationship between the duration of experiment (t), thermal diffusivity (s) of medium and a fraction (p) of the total energy produced by the infinite line source and stored within a distance (d):

$$d^2/(4\ st) = (p - 1 + e^{-d^2/4st})/\ E_1\ (d^2/4st) \qquad \textbf{(2)}$$

where E_1 is an exponential integral function. The dependence of $d^2/4st$ vs. p is given in Fig. 5. For instance, assuming an energy fraction of 90 %, thermal diffusivity of $1.0 \cdot 10^{-6}$ $m^2\ s^{-1}$ the distance d is 2.3 cm for 100 s, 7.2 cm for 1000 s, 22 cm for 10000 s, and 72 cm for 100 000 s. Thus a duration of measurement of more than a day is still providing a response from a distance less than 1 m away from the borehole. In order to reach the scale of 8 - 25 m, as discussed above on the basis of current repository planning, the duration of the measurement should be in the approximate range of 150 days - 4 years, respectively. It is evident, that in practice the scale of measurement cannot be increased infinitely by increasing the duration of measurement. The same restrictions would apply for cross-hole measurements: for such a measurement to be practical, the boreholes should be at a relatively short distance from each other.

The practical realizations of *in situ* probes are always finite cylinders, and the infinite cylinder/line source condition is never met with. In order to be a good approximation of the infinitely long source, the length/diameter ratio of the probe should be sufficiently big. This also depends on the duration of an experiment, as the axial losses increase in importance the longer is the experiment. According to Blackwell (1956) the ratio should be of the order of 25 to reach an uncertainty of only about 1 % in temperatures at the centre of the probe.

5.2 Case histories of applications

5.2.1 Investigations in boreholes in bedrock and soil

Beck et al. (1971) summarized a long experience in applying *in situ* measurements of thermal conductivity in boreholes in crystalline and sedimentary rocks in Canada. The applied principle of measurement was based on the solution of a perfectly conducting circular cylinder in an infinite homogeneous medium with a constant heat output from the cylinder. Beck et al. (1971) provided an analysis of the methods for deriving thermal conductivity with using an approximation of the solution for long times, which was typical for times when the numerical computing capacities were more restricted than today. In addition they used a visual curve fitting with numerically calculated response curves. This however, was found to be satisfactory for conductivity determination but not very useful for diffusivity due to the unknown value of contact resistance.

The applications built by Beck et al. (1971) were all designed for slim holes with diameters in the range of 35-57 mm. The constructed probes were relatively short and about 1 m long. Several technical alternatives for probe design were tested, and the best type was found to be a hollow metal (copper) cylinder. The heating wire was placed in a groove on the outer surface of the tube and the temperature sensors on the inner surface of the probe. In order to prevent convection in the hole, Beck et al. (1971) experimented with inflatable packers, as well as with simple 'bottle brush seals'. The latter were found to be practically as efficient as the packers. As a conclusion Beck et al. (1971) noted that the *in situ* probe method gives reliable results in a wide range of conductivities in both cased and uncased holes, given that the experiment duration is a couple of hours and that more than one method is used in derivation of the results. Considerable freedom can be allowed in probe materials and design if 10 % relative inaccuracy is sufficient, but reducing this to 3-5 % would demand much more careful probe design as well as revision of the method of interpretation.

Burkhardt et al. (1990, 1995) reported results obtained in the German super-deep drilling programme KTB. A thermal conductivity tool for measurements in the 4000 m deep KTB pilot hole was designed and tested. The operation principle of this probe was also the perfectly conducting cylinder with a constant heat power. Special attention was taken in the design to adapt the probe with the high viscosity drilling muds used in the borehole. Due to larger diameter of the hole (15 cm) the probe was made 3 m long with a nominal clearance of 3 cm. The tool was separated between inflatable packers. The experiment lasted typically 10 hours, which resulted in an influenced rock volume of c. 2.5 m^3 (corresponds to about 50 cm from the borehole centre), and the thermal conductivity was determined using the linear approximation for long measurement times. The derived conductivity values as calculated from the temperature sensors at 6 different positions along the probe show higher values towards the ends of the probe, which can be attributed to the axial losses. The deviations between centre and end sensors was about 0.5 W m^{-1} K^{-1}, but the conductivities calculated using the temperature curves recorded in the centre where mostly within 0.1 W m^{-1} K^{-1} of the laboratory measurements of the corresponding core samples (Fig. 6).

Behrens et al. (1980) used a packer-separated cylindrical probe for *in situ* measurements in the Urach geothermal anomaly, Germany. The probe was 2 m long and designed for 51 mm holes, and the thermistor sensor was placed at the centre of the probe. A pump located at the lower part of the probe was used to circulate the water between packers to ensure complete mixing of water. Thermal conductivity was calculated from the linear approximation for long times from the infinite cylinder source solution. Heating times of up to 10 000 s were applied. The measurements were controlled with drill core samples taken at the same depths, and the comparison suggested that only about 10 % deviations occurred with the laboratory measurements yielding higher values.

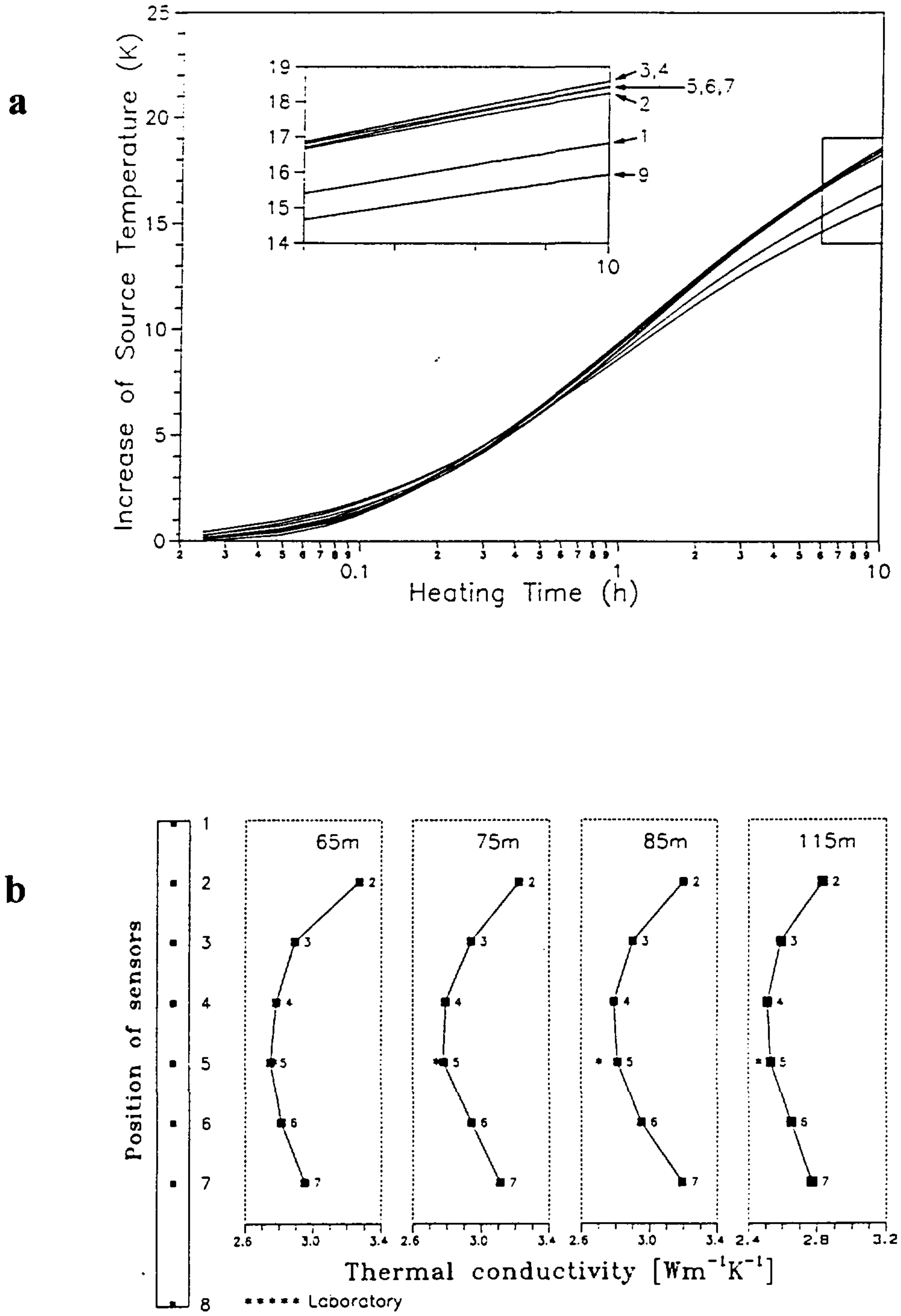

Figure 6. *a) Temperature records of the cylindrical continuous heating probe constructed by Burkhadt et al. (1995) in the KTB project, b) thermal conductivities determined at four depth values from temperatures responses of different temperature sensors.*

Kristiansen et al. (1982) described *in situ* measurements in very shallow holes drilled in outcrops of either Precambrian, Paleozoic and Mesozoic rocks on the island of Bornholm, Denmark. They applied a cylindrical hollow 0.42 m long probe with a diameter of 1.2 cm. Measurements were conducted either in water, grease or air filled holes with the same nominal diameter as the probe. One thermistor was placed at the central part of the probe and heating power was about 20 W m^{-1} through an insulated manganin electrical heating wire. Measuring times of up to 5000 s were applied, and thermal conductivity value was derived from the linear approximation for long measuring times. For crystalline rocks, the results were in a tight range, and they were also controlled from estimates based on mineral composition. The agreement was found to be good. Sedimentary rocks showed much more wider range in measured conductivity values.

Scroth (1983) presented a probe for simultaneous measurement of natural temperature gradient in the rock as well as thermal conductivity *in situ* measurement using the cylindrical source method. The probe (diameter 46 mm) was designed for use in shallow (<50 m) holes with a PVC casing (51 mm inner diameter). The convection of water was prevented with impermeable rubber lamellae placed along the probe. A 6 kg weight secured the smooth lowering and uplifting of the probe. Thermal conductivity was calculated from the typical linear approximations for long times but also from numerical finite difference modelling.

Yamada (1982) developed the derivation techniques of conductivity calculation from the cylindrical source solutions by studying the problem in the Laplace domain which made it easier to use a longer section of the temperature record than in the traditional linear approximation for long times. The probe design was comparable to others referenced above: a 1.2 m long (25.4 mm outer diameter) brass tube, tubular heaters and six thermocouples. The application was designed for very shallow holes and the thermal contact with the probe and hole was ensured with silicone fluid.

Tan and Ritchie (1997) used the linear source solution to determine thermal conductivities of mine waste rock piles. Their probe was 1.15 m long with an outer diameter of 36 mm. Heating was arranged with eight longitudinal nichrome wires supported on Teflon disks mounted at 0.15 m intervals on a steel rod. The heat power applied was 7.1 W m^{-1}. Tan and Ritchie (1997) measured the probe temperatures both during heating and cooling, and fitted results independently on both recordings using the linear approximations for long measurement times. Diffusivity was determined by fitting repeated temperature logs in 16 m deep holes and modelling of the downward propagation and damping of the annual temperature wave.

A similar method for determining the *in situ* diffusivity of the uppermost 30-50 m of bedrock was used by Parasnis (1974) in the Skellefte area in Sweden. The annual surface temperature variation was assumed to be sinusoidal and the bedrock was approximated as a homogeneous half-space. The thermal diffusivity was determined with a least squares method of fitting the model results with borehole measurements. The obtained values of thermal diffusivity were higher (by a factor of about 5) than typical values for crystalline rocks, but the difference was attributed to the sulphide mineralization of the rocks.

Mussmann and Kessels (1980) constructed a special probe for *in situ* thermal conductivity measurements. In their application a 30 cm long side hole (diameter 13 mm) deviating 30° from the main hole is drilled with a hydraulic drilling system. A sensor with a diameter of 12 mm is placed at the bottom of this hole. A spherical heater at the front end of the sensor produces a spherical temperature field, which is registered with eight thermistors along the sensor. From the geometry of the heater and its constant temperature the conductivity and diffusivity of the surrounding rock can be calculated. The method has not gained popularity, as far as the literature is reviewed, perhaps due to the technical complexity related to the combined drilling and measurement operations, and the disturbing effect of the side drilling system itself. In addition the scale of investigation is not essentially larger than when using representative core samples.

Sass et al. (1981) developed a technique for measuring thermal conductivity and temperature gradient effectively *in situ* in unconsolidated sediments. The measurement is done during a drilling break by pushing hydraulically a thin (6 mm outer diameter) 1.5 - 2.0 m long probe into the sediments through the drill bit (Fig. 7). Temperature is recorded with three thermistors placed at 0.15-0.5 m apart and temperature gradient is determined after 25 minutes of waiting time. A line source heater is switched on and thermal conductivity is measured using a 15 minute heating period. The calculation is done with the linear approximation for long times. The technique was found to be cost-effective in exploration for geothermal resources (high heat flow areas), because no casing, grouting or hole monitoring after drilling is needed. The method can be used only in reasonably soft, unconsolidated sediments. It is analogous to typical marine heat flow measurements.

Direct *in situ* measurements of heat flow density have been developed for many applications and these are usually based on placing a probe with known conductivity in the medium of interest. From a measurement of the temperature gradient in the probe, and a geometrical factor depending on the shape of the probe, the heat flow density can be determined. In other applications than borehole geophysics a thin plate oriented perpendicular to the heat flux is typically used. Theoretical solutions are available for oblate ellipsoids oriented either perpendicularly (Philip, 1961) or parallelly (Carslaw and Jaeger, 1959) to the flux. One application was described by Oelsner and Rösler (1981) who used a combination of two probes with very different conductivities (aluminium, 155 W m^{-1} K^{-1}, and 'Hartgewebe', 0.26 W m^{-1} K^{-1}). Oelsner and Rösler (1981) did not yet report any practical results.

Jolivet and Vasseur (1982) presented a method of measuring directly heat flow density *in situ* in boreholes. In this method a probe with a heat source in the upper and a heat sink in the lower end of a probe are used. The source-sink pair produces a heat flux which is opposite to the geothermal heat flux. The heat source and sink, which have equal values but opposing signs, are adjusted so that the temperatures at the ends of the probes are equal. In stationary conditions the value of applied source (sink) value depends only on the ambient heat flow density and probe geometry. Once the geothermal heat flow density is known, the thermal conductivity can be calculated with the aid of a temperature gradient value, which can be measured immediately before the heat flow density. In practice, the method demands numerical simulations for the interpretation.

A number of methods is based on using the heating (alternatively cooling) effect of the drilling fluid which often has a temperature different than the formation. Theoretically the methods are very close or analogous to the cylindrical source method with the major difference in the realization of the heating technique and using the transient after heating for conductivity determination. The thermal relaxation of the borehole wall is assumed to have preceded by a period of constant heat flow across the boundary (during the drilling time), and the fluid conductivity is assumed to be perfect (Blackwell, 1954). There is a considerable literature (see, e.g., Haenel et al., 1988 for a summary) on estimating the

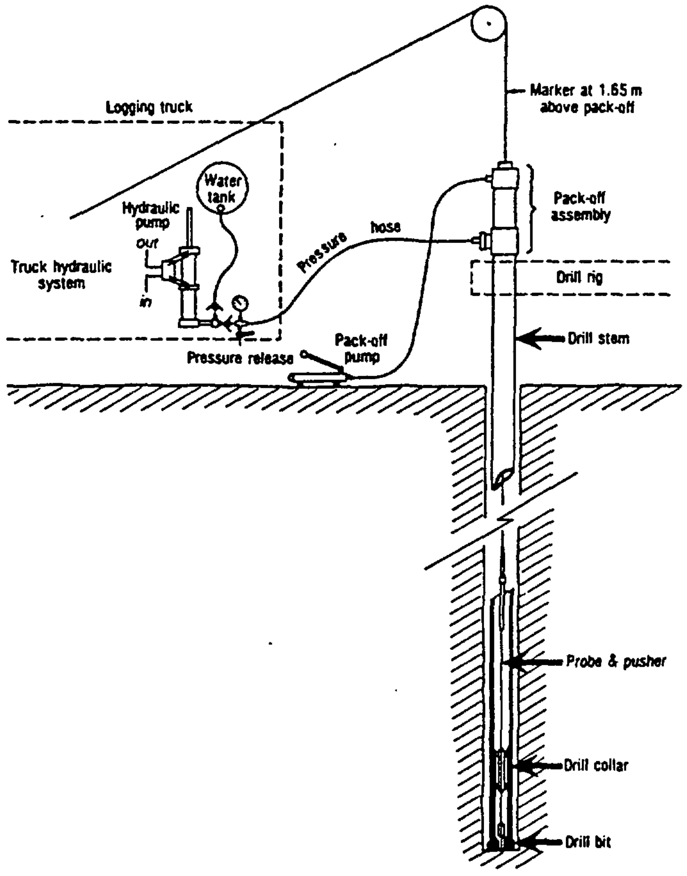

Figure 7. *System designed for measuring thermal conductivity in situ in soft sediments during drilling (Sass et al., 1981).*

undisturbed borehole temperature from a series of transient logs of temperature in a borehole, because such a measurement situation is typically encountered in logging of temperature gradients in geothermal studies of oil wells. Using of the transient temperature behaviour of a borehole to thermal conductivity estimation is reviewed shortly by Wilhelm (1990) who also presented a method independent of the knowledge of the heating history, and only the temperature logs would be needed. In practice, the constant heat flow condition is not often realized. In Wilhelm's method, Marquardt inversion was used for estimating the initial temperature disturbance in the hole, undisturbed temperature of the rock and the heat capacities of the rock and borehole fluid for a given values of thermal diffusivities. A case history presented by Wilhelm (1990) indicated very low values of determined conductivity *in situ*, which was attributed to the convective fluid movements in the open hole.

Xu and Desbrandes (1990) used a similar technique but they monitored also the temperature at a depth of interest during the fluid circulation. The temperature vs. time was solved with numerical solution of the heat conduction equation including fluid storage effects analogous to drawdown tests of wells. A crossplot technique for formation evaluation was developed using volumetric heat capacity and thermal conductivity.

Sundberg (1988) described a multi-probe method for thermal conductivity and diffusivity determinations of soils in Sweden. The application tested in shallow (20 m) holes was using a line source approximation for conductivity calculation. In contrast to the many applications of single hole methods, Sundberg (1988) used also two parallel shallow holes at a distance of 6-20 cm from each other. In one hole a heater probe (1.2 m long) is used and temperature is measured with time in the other hole (probe length 0.6 m). Constant heating power and infinite line source approximation were used. However, no detailed report of the *in situ* measurement was given by Sundberg (1988) perhaps due to technical problems.

5.2.2 Marine and lacustrine geothermal studies

Measurement of geothermal heat flow density at the bottoms of seas and lakes is usually not based on drilling holes for gradient and thermal conductivity measurements. Instead, a penetrating probe is pushed to the soft bottom sediments, and the temperature gradient is measured with a number of temperature sensors placed along the probe. A heat pulse is generated with a line source heater and the transient response is used for thermal conductivity determination. In oceanic bottom at water depths exceeding 2000 m the bottom temperature is very stable and the geothermal gradient can be measured in the uppermost few metres of the bottom sediments. In lakes and shallow seas the situation is different and long period temperature monitoring may be needed to remove the disturbances of the variations in bottom temperatures (Beck and Shen, 1985) .

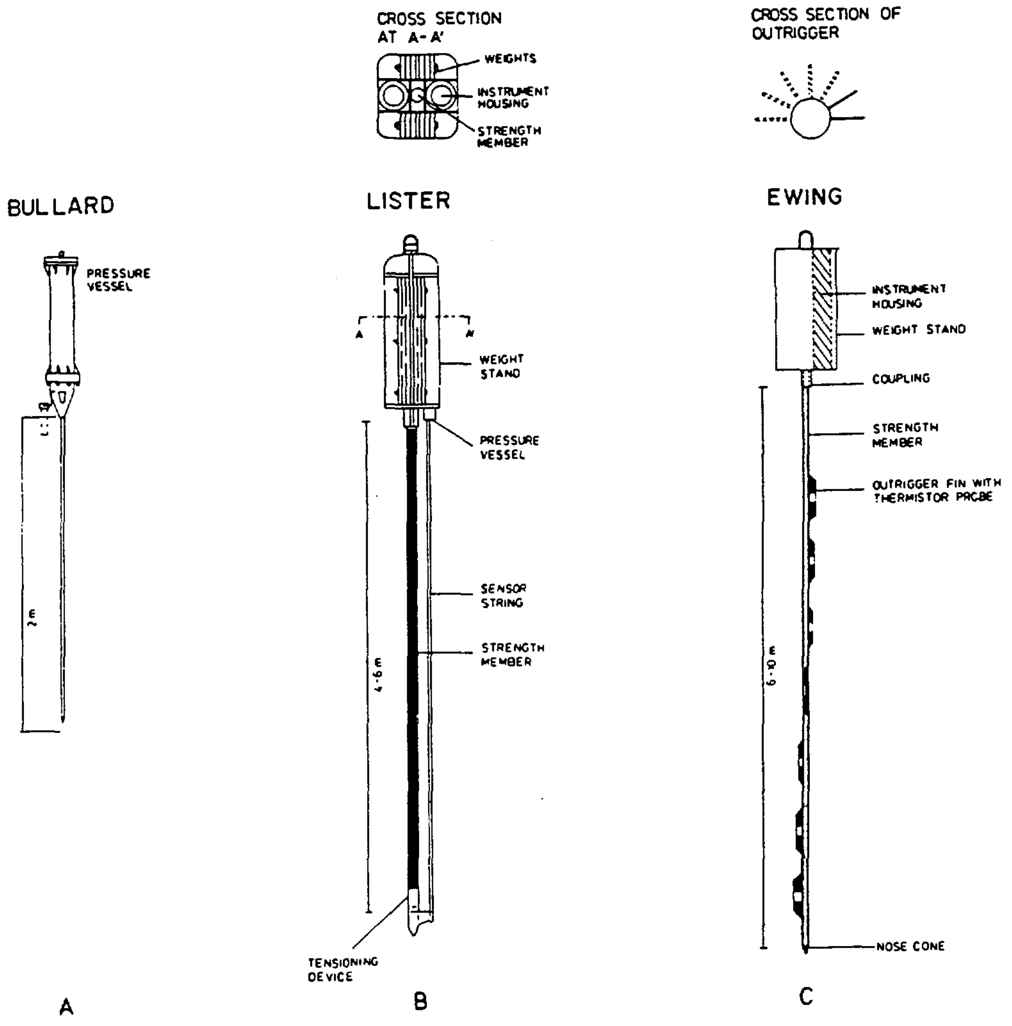

Figure 8. *Different types of heat flow probes used in geothermal studies of oceanic areas (Louden and Wright, 1989).*

The temperature and thermal conductivity instruments are mounted in sensor strings either inside of a mechanically strong rod (strength member) or next to it. Three main probe types have been used: Bullard, Lister and Ewing probes (Davis, 1988) (Fig. 8). The Bullard probe is the oldest construction, and it has a penetrating probe of 2m length. The temperature sensors (thermocouples) and heating wires are installed in the strength member with a diameter of 1.0 cm. The relatively large thermal inertia of the probe resulted in long measurement times of about 30-50 min after the penetration. In the Ewing probe the thermistors and heating wires were installed in outrigger fins at a distance of about 10 cm from the strength member, and the thermal conductivity probe diameter is only 0.4 cm. In the Lister (or 'violin bow') probe, the sensor string is installed in a separate thin rod at a distance of about 10 cm from the strength member. A heavy weight on top of the strength members ensures the penetration to the sediment.

Thermal conductivity is usually determined from a transient response to a short heat pulse (Lister, 1979), but also continuous heating systems have been applied (Bullard, 1954; Hyndman et al., 1979; Davis, 1988). The heating and measurement times are usually in the scale of 5-15 minutes. The smaller is the diameter of the thermal conductivity probe, the shorter measurement times can be applied. The probe diameters are typically 0.16 - 1.0 cm (Jemsek and von Herzen, 1989). Also the frictional heating by the penetrating probe has been used for thermal conductivity measurements (Bullard, 1954; Kalinin, 1983).

Measurements in lakes are technically similar to the marine measurements (Haenel, 1979), although the probes used are usually of a lighter construction. Measurements in Scandinavia have been reported by Haenel et al. (1979) and Lindqvist (1983, 1984) and in Canada by Allis and Garland (1976).

5.2.3 Lunar studies

The investigation of the Moon during the Apollo program in the 1960-70's included also heat flow studies, and on Apollo 15 and 17 missions, thermal instrumentation was installed at shallow depth in the lunar regolith soil (Langseth et al., 1972, 1976; Langseth and Keihm, 1977). Thermal conductivity was determined *in situ* with a 1 m long probe of 2.5 cm in diameter pushed into the soil with a drillstem. Temperature was measured with four platinum thermistors at 20 - 30 cm distances of each other. In the middle of the thermistors there was a short heating wire as a heat source (0.002 W). The heat source was kept on for 36 hours and the temperature change in the thermistors was recorded. Thermal conductivity was calculated using either the analytical solution of a spherical constant heat source or using a numerical finite difference simulation of the experiment. The lunar problem is complicated by the unknown contact resistance at the probe/soil interface as well as the very low soil conductivity (of the order of 0.01 W m^{-1} K^{-1}) which resulted in long recording times in comparison to terrestrial measurements. The low conductivity can be attributed to the vacuum and the high porosity of the soil produced by continuous 'gardening' by the meteoritic bombing. Even the 36 hours of duration of experiment was able to represent conductivity only to a distance of about 2-3 cm from the probe.

5.2.4 Indirect estimation methods of in situ thermal properties

Thermal properties can be estimated also indirectly with the aid of other parameters related to thermal conductivity and diffusivity. Such applications are naturally related to borehole investigations.

Williams et al. (1988) investigated the Cajon Pass scientific drill hole near the San Andreas Fault in California, and estimated thermal conductivity of the intersected granitoid rocks from geochemical logs. These logs, based on both natural and induced spectroscopy logs, yield data on the concentrations of Al, Si, K, Ca, Fe, S, Ti, Gd, U, Th and Na+Mg sum, and they can be used for calculating the mineralogical composition of the rocks. Geometric mean of mineral conductivities was then used to obtain a profile of thermal conductivity. Comparison with the few core samples in the studied hole section gave confidence that the estimated conductivity matches reasonably well with sample data, and the negative correlation of estimated thermal conductivity and temperature gradient suggests that the gradient changes are due to conductivity changes and not to small-scale fluid circulation in the hole. Mainly this can be attributed to conductive heat transfer, because heat flow density is the product of conductivity and gradient.

Brigaud et al. (1989) determined thermal conductivity of sedimentary rocks in oil wells using a technique based on various geophysical well logs for porosity and lithological type estimation (resistivity, density, sonic, neutron and gamma ray logs) and correlations between thermal conductivity vs. porosity and thermal conductivity vs. content of a given lithotype in the rock (i.e., clay, quartz or carbonate content). Thermal conductivity was estimated with geometric mean values of various contributing elements (Fig. 9). Brigaud et al. (1990) used also laboratory measurements to determine the rock matrix thermal conductivity of different lithofacies samples (cuttings). After determining the porosity and relative proportions of different lithotypes with well logs, a geometric mean model was applied to obtain thermal conductivity. The estimated thermal conductivity is considered to be correct within 20% of the correct values. This kind of estimation techniques are necessary in oil drilling, because drill core samples are rarely taken.

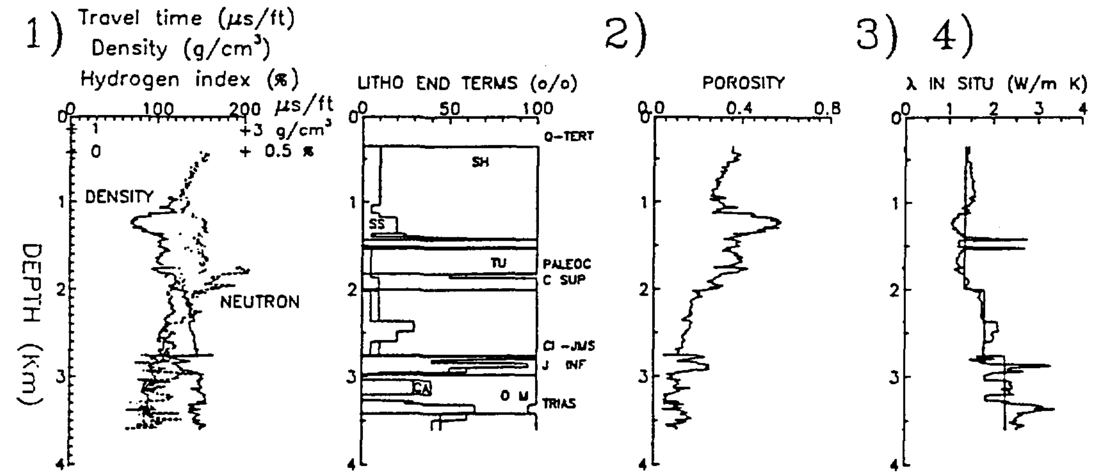

Figure 9. *Indirect estimation of thermal conductivity in situ with the aid of geophysical logs and lithological data from cuttings (Brigaud et al., 1989).*

Williams and Anderson (1990) used well-logs for estimating thermal properties (conductivity and heat production rate) *in situ* in boreholes in the continental and oceanic crust. With the aid of a phonon conduction model and well-log derived estimates of mineral composition combined with known mineral conductivities as well as well-log derived density, seismic velocities and porosity, it is possible to predict thermal conductivity within ±15 %. Anisotropy and fracturing remain problems limiting the achieved accuracy.

Estimation of thermal conductivity of crystalline rocks was investigated by Pribnow et al. (1993) in the German super-deep drilling program KTB. In the fully cored 4 km deep KTB pilot hole, a comprehensive comparison of core measurements in laboratory and well-log derived estimates of conductivity was carried out. A phonon conduction model similar to that used by Williams and Anderson (1990) was used. Since thermal (phonon) conductivity of solids is proportional to density, specific heat capacity, phonon velocity and phonon mean path, the thermal conductivity can be estimated with these parameters with the aid of well-logs. The results in the KTB case indicated that the method is accurate in the case of isotropic or flat-lying anisotropic crystalline rocks. However, anisotropic gneisses with varying dip angles of foliation showed significant differences between core and well-log derived estimates.This was attributed to the presence of microcracks in the core samples, anisotropy of the thermal conductivity of mica and problems of measuring reliably the shear wave velocity in the borehole in the presence of significant dipping anisotropy.

5.2.5 Full scale in situ experiments related to nuclear waste and other studies

The heating effect of the spent nuclear fuel canisters produces thermal loading of the surrounding rock mass. The resulting thermal expansion creates stress field variations, and deformation of the rock mass may also take place. There may also be changes in hydraulic permeability due to fracture dilatation or formation of new fractures. These effects can be analysed with theoretical models (e.g. Hodgkinson and Bourke, 1978; Cook and Witherspoon, 1978) but also with full scale experiments. Such investigations have been carried out in various rock environments, including basalt (Hocking et al., 1981), granite (Bourke et al., 1978; Kuriyagawa et al., 1983), and salt (Kopietz and Jung, 1978; Rotfuchs, 1978). These experiments which were all carried out by placing electrical heaters in boreholes and measuring the temperature increase and other related effects in surrounding boreholes. The slow conduction of heat in rocks usually limits the time span of such experiments, and the measurements have usually been done within the nearest 15 m from the heaters, and results are available only for short times of the experiments.

Thermal conductivity *in situ* was usually not the prime target in such experiments and the conductivity has been typically determined with forward modelling of the conductive heat transfer in the situations investigated. Such an approach is complicated by the fact that thermal conductivity is temperature dependent and in details it is usually unknown for a given formation. Therefore, if very high heating powers are used (e.g. Kuriyagawa et al., 1983, whose heater hole temperature was as high as 440°C) the determination of conductivity becomes more complicated. The situation is also influenced by the thermal contact resistance and others than conduction dominated heat transfer mechanisms (convection, vapour diffusion, radiation) in the heater holes.

Chan and Jeffrey (1983) reported results of thermal parameter estimation with an *in situ* heating experiment in the Stripa mine, Sweden. An electrical heater imitating the heat generation of a nuclear waste canister was placed in a borehole at a depth of 4 m from the drift floor and temperatures were monitored with about 20 thermocouples in surrounding holes (Fig. 10). The thermocouples were all within 3-4 m of the heater. The heating period lasted 70 days, and temperatures were followed altogether for 140 days. The temperature field during heating and cooling was modelled with a finite line source model, and inversion of the measured temperatures for conductivity and diffusivity was done using a non-linear multivariate regression model based on Green's function solution. The sensitivity analysis of the inversion parameters suggested that conductivity and diffusivity are well identifiable, and comparison with laboratory measurements on core samples indicated values deviating less than 5 % (conductivity) and 13 % (diffusivity).

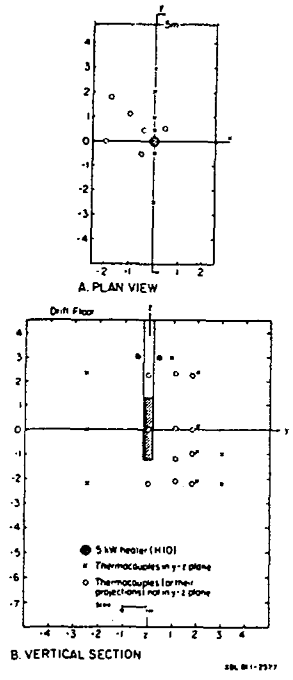

Figure 10. *The arrangement of in situ measurement of thermal conductivity and diffusivity in the Stripa mine, Sweden (Chan and Jeffrey, 1983).*

Chan and Jeffrey (1983) discussed also the scaling problem of thermal conductivity, particularly in relation to fractures, which cannot be 'sampled' in a representative way in drill cores. Using forward models of effective thermal conductivity of rock with idealized fracture geometries, they noted that for rocks with water-filled fractures, the effective thermal conductivity is within a few percent of the rock matrix value for any assumed fracture geometry. Models with air-filled fractures showed more deviation, but only if the solid-solid contacts were assumed inefficient.

5.3 Discussion on the applied methods with a reference to nuclear waste disposal studies

The surveyed literature suggests that there are two main ways of determining thermal properties *in situ*. These are either the transient single hole measurements with a cylindrical (or linear) heat source, or indirect estimation of conductivity from other borehole data and cuttings.

The popularity of single hole methods in measurement of thermal parameters is due to the low diffusion rates of thermal signals in rocks. In practical applications it is not feasible to wait the very long times needed to receive a thermal signal from a neighbouring borehole at a distance of more than a few metres. Case histories of multiple-hole measurements have been conducted only in special cases, and the measurements are dependent on local circumstances. However, there would be no principal obstacles for designing *in situ* measurements of thermal properties between canister holes during the construction stage of the final repository. At a hole distance of 8 m, the experiments would have a characteristic time of about a year. However, such measurements could not anymore be used in planning the placing and exact distances between the canister holes.

The indirect estimation techniques based on a combination of well-logging and mineral composition data are applicable in cases where such data is available. The representative volume of such measurements depends on the applied well-log methods. The penetration depth of different methods varies, but in most methods used it is within a few to few tens of centimetres from the hole. In the Finnish nuclear waste investigations, methods such as those used by Pribnow et al. (1993) or Williams et al. (1988) would not essentially increase the level of information because all deposition holes will probably be sampled using coring. Therefore, the effort should be put in methods enlarging the volume of investigation in relation to laboratory measurements of drill cores.

One relatively simple method of thermal conductivity estimation can be based on a passive measurement of the natural temperature gradient using a high temperature resolution. Since geothermal heat flow density can be assumed to be constant at least locally in a drill hole, the measured gradient changes can be attributed to thermal conductivity variations (heat flow density is a product of gradient and conductivity). Then, a temperature gradient log can be transformed into a log of 'apparent' thermal conductivity, which can be calibrated with drill core measurements. However, the temperature gradient changes are not only due to thermal conductivity variations in the scale of the drill core, but reflect also larger scale variations in rock texture and anisotropy surrounding the borehole. Thus, a comparison of the 'apparent' thermal conductivity and drill core samples provides a means to estimate the representativity of the core sample measurements in relation to larger volumes.

Since average heat flow density in the Finnish bedrock is about 37 mW m^{-2} (Kukkonen, 1989), and rock conductivity is between 2 and 5 W m^{-1} K^{-1}, the gradient values could be expected to vary by a factor of about 2, between 7 and 18 mK m^{-1}. To measure such gradient changes in a drill hole at a scale comparable to drill core samples (10 cm), a resolution of about 0.1 mK would be needed, which would be technically rather demanding. In the scale of metres, a resolution of about 1 mK would be sufficient. This is possible already. But such a measurement could be disturbed by water flow in the hole, and the temperature measurement should preferably be done between packer-sealed sections to secure the recording of conductive gradients.

At the moment, the most feasible method for *in situ* measurement of thermal conductivity seems to be an active single-hole system based on a transient response of a cylindrical heat source. This is supported by several factors: (1) the scale of measurement can be controlled by the length of probe and time duration of the experiment, (2) a wide range of conductivities can be measured, (3) both conductivity and diffusivity can be determined in a single experiment, (4) mathematical devices are available for the inverse solution in the basic cases, (5) drill hole may be cased or uncased, and (6) there is a lot of literature of using such methods. Therefore, we suggest that the preliminary design of a measurement system should be based on this method.

6 NUMERICAL SIMULATIONS

In the following, we present results of forward and inverse simulations of a theoretical single-hole system with the aim of understanding the relevant factors related to such measurements. The theoretical models for the probe are a perfectly conducting circular cylinder with infinite length and a finite length line heater, which are located in an infinite medium. The infinite cylinder model is here used to study the conduction of heat caused by heating of the probe. This model is considered to be a reasonable model for basic analysis of the anticipated measurement system (Kristiansen, 1982). The thermal contact resistance is taken account in the model, which is essential for practice, as the contact resistance cannot be avoided in any probe design. The effect of the finite length of the true probe is studied using simulations with a line heat source. The heating is assumed to be continuous or a pulse-form signal. The temperature rise is calculated in the probe, as well as in the surrounding medium.

Using an infinite cylinder model synthetic sets of measurements were generated. These (with Gaussian noise added) data were then interpreted using the same model to simulate the realistic borehole measurements and to find a good heating and measuring practice. The geological parameters to be estimated were conductivity and diffusivity. Also the thermal contact resistance was assumed to be unknown and estimated from the measurements.

The parameter estimation problem was solved as a nonlinear least squares problem. Different measurement times and pulse lengths were considered, and the effective radius of measurements was estimated as well. In addition, the sensitivity of estimation accuracy affected by erroneous measurements was investigated.

The following symbols and units were used:

λ = rock thermal conductivity [W m^{-1} K^{-1}],
λ_W = water thermal conductivity [W m^{-1} K^{-1}]
s = rock thermal diffusivity [m^2 s^{-1}],
ρc = density×specific heat [J m^{-3} K^{-1}], calculated by λ/s,
a = the effective radius of the probe [m],
Q = power input of the probe/ unit length [W m^{-1}],
H = 1 / thermal contact resistance [W m^{-2} K^{-1}] = λ_W / d
= conductivity / thickness of the contact layer between probe and rock,
S = effective heat capacity of the probe/unit length [J m^{-1} K^{-1}],
t = time [s],
b = length of the line heater [m],
r = radial coordinate in cylindrical polar system [m],
z = vertical (axial) coordinate in cylindrical system [m].

6.1 Theoretical models

The theoretical cylinder model is used here to study the conduction of heat caused by heating the probe. A perfectly conducting circular cylinder with infinite length is located in an infinite medium. It is assumed that the (rock) medium is continuous, isotropic and homogeneous. The temperature rise of the cylinder (probe) which is producing heat at a constant rate is given by (Jaeger, 1956)

$$v(t) = \frac{2\alpha^2 Q}{\lambda\pi^3}\int_0^\infty \frac{1-\exp(-\tau u^2)}{u^3\Delta(u)}\,du \tag{3}$$

where

$$h = \frac{\lambda}{aH}, \quad \alpha = \frac{2\pi a^2 \rho c}{S}, \quad \tau = \frac{st}{a^2}, \tag{4, 5 \& 6}$$

and

$$\Delta(u) = [uJ_0(u) - (\alpha - hu^2)J_1(u)]^2 + [uY_0(u) - (\alpha - hu^2)Y_1(u)]^2. \tag{7}$$

The $J_n(u)$ and $Y_n(u)$ are the Bessel functions of the first and second kinds and order n.

The infinite integral solution for the temperature increase $v(t)$ has been approximated at large and small times (e.g. Jaeger, 1956). The large time expression is approximately:

$$v(t) = \frac{Q}{4\pi\lambda}\{[2h + \ln(\frac{4\tau}{e^\gamma})] - \frac{(4h-\alpha)}{2\alpha\tau} + \frac{(\alpha - 2)}{2\alpha\tau}\ln(\frac{4\tau}{e^\gamma}) + \cdots \tag{8}$$

where γ is Euler's constant (0.5772). The $v(t)$ versus ln t is asymptotic to a straight line with slope $Q/4\pi K$ and intercept $I = \ln(e^\gamma a^2/4s) - 2h$ on the ln t axis. This linear asymptote is used to estimate both conductivity λ and diffusivity s. It is noticed (e.g. Jaeger, 1958) that small error in the slope will lead to larger error in the intercept. In using the linear asymptote to estimate the diffusivity s, the contact resistance $1/H$ should be known.

When the cylinder (probe) is producing heat at a constant rate the temperature rise in the external medium ($r > a$) is given by (Jaeger, 1956):

$$v(r,t) = \frac{\alpha Q}{\lambda \pi^2} \int_0^\infty \frac{[1-\exp(-\tau u^2)]\{J_0(ru/a)[uY_0(u)-(\alpha - hu^2)Y_1(u)] - Y_0(ru/a)[uJ_0(u)-(\alpha - hu^2)J_1(u)]\}}{u^2\Delta(u)}\, du, \tag{9}$$

where h, α, τ and $\Delta(u)$ are as before.

The temperature rise due to a constant power finite length line heater is given by (Chan and Jeffrey, 1983):

$$v(r,z,t) = \frac{Q}{4\pi\lambda} \int_0^b \frac{\operatorname{erfc}\left[\frac{\sqrt{r^2+(z-z')^2}}{2\sqrt{st}}\right]}{\sqrt{r^2+(z-z')^2}}\, dz', \tag{10}$$

where 'erfc' refers to the complementary error function. This solution assumes that the line heater is in direct thermal contact with the rock (H=∞) and the heater and rock have the same thermal properties. This expression is used to simulate the temperature increase in the external medium (in cylindrical polar system). The thermal power of the line heater is $Q \times b$.

The special functions J_n (u), Y_n (u) and erfc( ) are calculated using IMSL MATH/LIBRARY™ special functions. The integrals above are calculated numerically using IMSL subroutines *dqdagi* and *dqdag* of the same library.

The pulse heating is calculated using superposition. If the continuous heating is stopped at the time moment t_1, the temperature response at $t > t_1$ is $v(t) - v(t-t_1)$. Turning off the heating is equivalent to having two 'identical' heaters, with the powers Q and $-Q$ and the operation times t and $t-t_1$. The needed response components at the time sequence needed are calculated by interpolating the continuous heating response curve using IMSL subroutines *dbsnak*, *dbsint*, *dbs1gd*). The relative error of the combined response function $v(t)$ is less than 10^{-5} (the number of "good" digits are at least 5), which is good enough for solving nonlinear least squares problems.

6.2 Interpretation of measurements

Conductivity λ and the diffusivity s of the rock are the geological parameters to be estimated from measured temperature variations in the probe. The thermal contact resistance is assumed to be unknown as well, and it must be estimated from the measurements. The parameter estimation problem is solved as a nonlinear least squares problem. In the interpretation the whole temperature record is used for obtaining maximum utilization of measurements (cf. Jaeger, 1959). The model for this inversion is the function of the temperature rise in a cylinder $v(t, \lambda, s, H, a, \ldots)$ (1). The measure M to describe the goodness of the model is:

$$\min M = \min_{p} \| \boldsymbol{v}(\boldsymbol{t},\boldsymbol{p},\boldsymbol{x}) - \boldsymbol{m}(\boldsymbol{t}) \|^2 , \tag{11}$$

where $\boldsymbol{p}$ is the vector of the m parameters to be estimated, $\boldsymbol{x}$ are the known model parameters and $\boldsymbol{m}(\boldsymbol{t})$ are n measurements at the time sequence $\boldsymbol{t}$.

To minimize the measure the trust region Levenberg–Marquardt optimization method is applied. The Levenberg–Marquardt method locally approximates the given nonlinear problem with the linear least squares problem. The optimization process iteratively adjusts the value of $\boldsymbol{p}$. The trust region strategy controls the step size of $\boldsymbol{p}$. Here *ODRPACK* - subprograms (Boggs et al, 1989) were used to solve the nonlinear least squares problem. In every iteration the Jacobian matrix $\partial v(\boldsymbol{t},\boldsymbol{p},\boldsymbol{x})/\partial \boldsymbol{p}$ was computed. It is the matrix $(n \times m)$ of first partial derivatives of $\boldsymbol{v}(\boldsymbol{t},\boldsymbol{p},\boldsymbol{x})$ with respect to each component of $\boldsymbol{p}$. In this study it was computed using finite differences of evaluated function $\boldsymbol{v}(\boldsymbol{t},\boldsymbol{p},\boldsymbol{x})$, although it could be computed faster using analytically differentiated expression of $\boldsymbol{v}(\boldsymbol{t},\boldsymbol{p},\boldsymbol{x})$. However, this does not contribute to the results. The used program calculates the linearized error estimators and correlation matrices of the estimated parameters.

6.3 Theoretical temperature responses

A set of forward solutions with different parameter values is given in Fig. 11-23. The parameters were chosen so that the results correspond to a situation of making an *in situ* measurement in a 56 mm drill hole. The probe diameter was assumed to be 42 mm. Thermal conductivity, diffusivity and the thermal contact resistance between the probe and the drill hole wall were varied in the simulations. The values of the contact resistance were guided assuming that the layer is either water or air and that heat transfer through the layer is conductive. The value of $H = 85.71$ corresponds to a situation where the contact layer is 7 mm thick and has the thermal conductivity of water (0.6 W^{-1} m^{-1} K^{-1}). In choosing the rock conductivity and diffusivity values it was assumed that these parameters are correlated (eq. 1), and an experimental relationship based on laboratory measurements of rocks from the Finnsih investigation sites (Kukkonen and Lindberg, 1998) was used:

$$s = 0.53\,\lambda - 0.2 \tag{12}$$

where λ is expressed in W $m^{-1}K^{-1}$ and s in 10^{-6} m^2 s^{-1}. The specific heat of the probe was assumed to be identical to a 42 mm outer diameter copper tube (2 mm wall thickness) filled with water. Continuous heating with a power of 20 W m^{-1} was used. Results for any other power value can be estimated from these results as the temperature increase is linearly proportional to the heating power.

The advantage of using the full numerical solution of the forward problem instead of approximations (eq. 8) is demonstrated in Figs. 11-14. It is evident, that even the almost linear parts of the responses could be misinterpreted if approximations were used.

For a given contact resistance the response curves are indistinguishable up to measurement times of a few hundred seconds (Fig. 15-18). This is due to the fact that the response comes first from the contact layer, and only after the heating starts to affect the rock the curves start to differ depending on conductivity. The slopes of the linear parts of the curves are good indicators of conductivity. When the contact resistance decreases (H increases) the shape of the curves is modified, and the surrounding medium beyond the contact layer is seen earlier in the response. However, the 'linearity' of the response for long times is influenced by the contact resistance in such a way, that cases with low contact resistance are less disturbed by this effect (Fig. 19).

Forward simulations of the pulse heating case are given in Figs. 20-23 (log time scales) and 24-28 (linear time scales). With respect to conductivity values, they are analogous to the continuous heating case, with the amplitude of heating increasing with decreasing conductivity. The temperature starts to decrease very sharply when the heating is turned off, which can be attributed to the infinite conductivity used in the solution of the heat conduction equation, and the temperature being measured in the heat source itself.

Different measurement times and pulse lengths were considered in the simulations. The pulse length was varied from 100-5000 s, and the cooling was simulated equally long times. Here again, the thermal contact resistance dominates the results in measurement and pulse times shorter than about 1000 s.

Generally, it can be seen that the temperature changes with the applied parameter values are a few K for measurement times of 10000 - 100 000 s. Such an amplitude would be reasonable considering practical measurements, and avoiding the influence of the temperature dependence of thermal conductivity on the results.

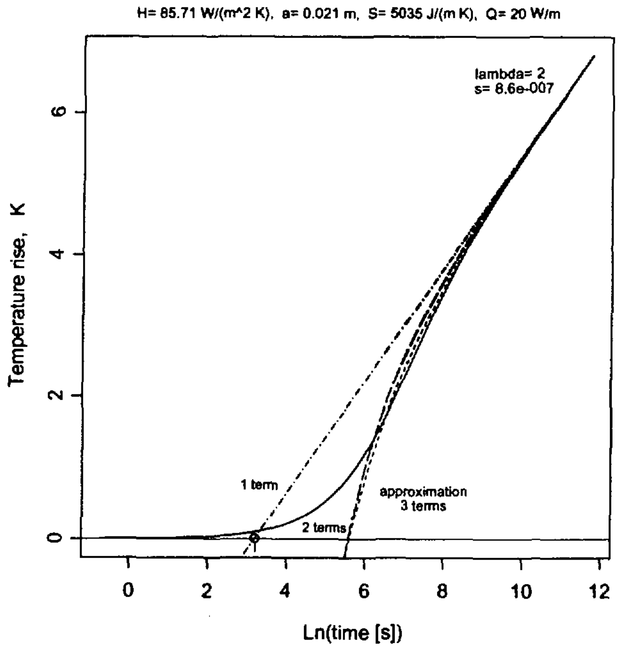

Figure 11. *Theoretical responses of the infinite cylinder probe with different numbers of terms included in the approximate solution and comparison to the 'correct' numerical solution. Conductivity of rock is 2.0 W m^{-1} K^{-1}.*

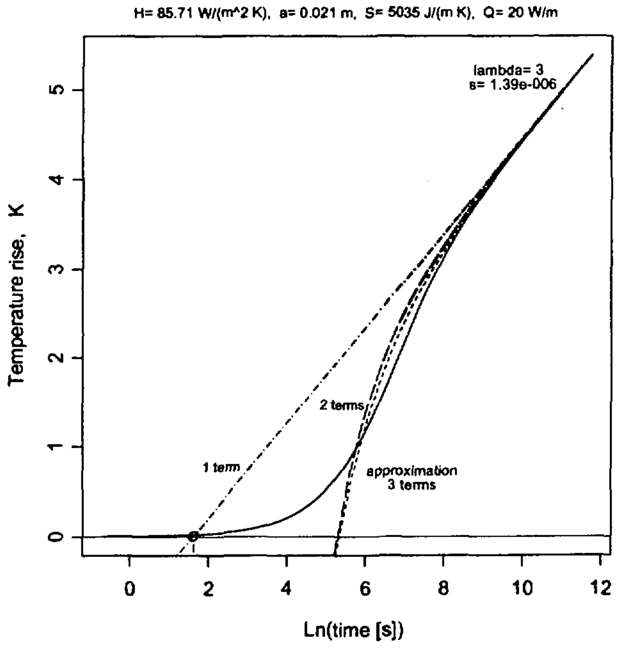

Figure 12. *Theoretical responses of the infinite cylinder probe with different numbers of terms included in the approximate solution and comparison to the 'correct' numerical solution. Conductivity of rock is 3.0 W m^{-1} K^{-1}.*

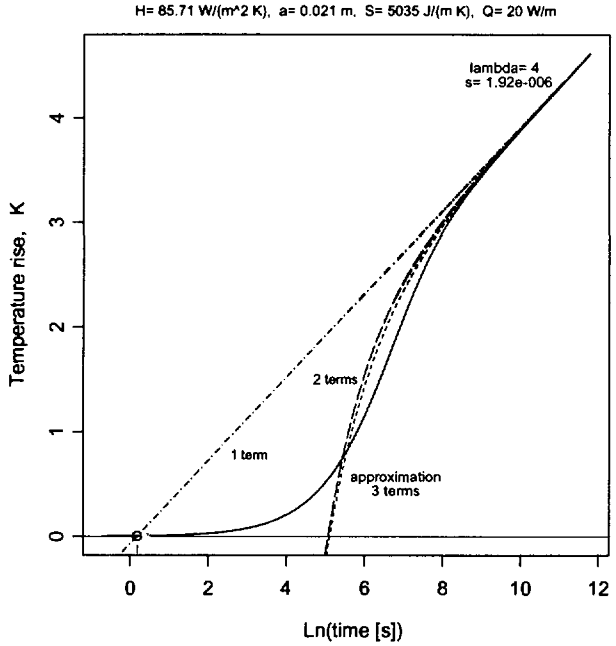

Figure 13. *Theoretical responses of the infinite cylinder probe with different numbers of terms included in the approximate solution and comparison to the 'correct' numerical solution. Conductivity of rock is 4.0 W* m^{-1} K^{-1}.

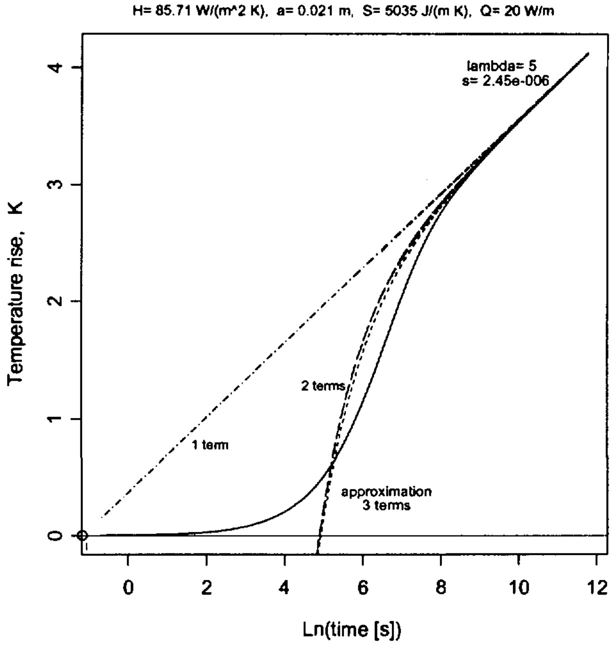

Figure 14. *Theoretical responses of the infinite cylinder probe with different numbers of terms included in the approximate solution and comparison to the 'correct' numerical solution. Conductivity of rock is 5.0 W* m^{-1} K^{-1}.

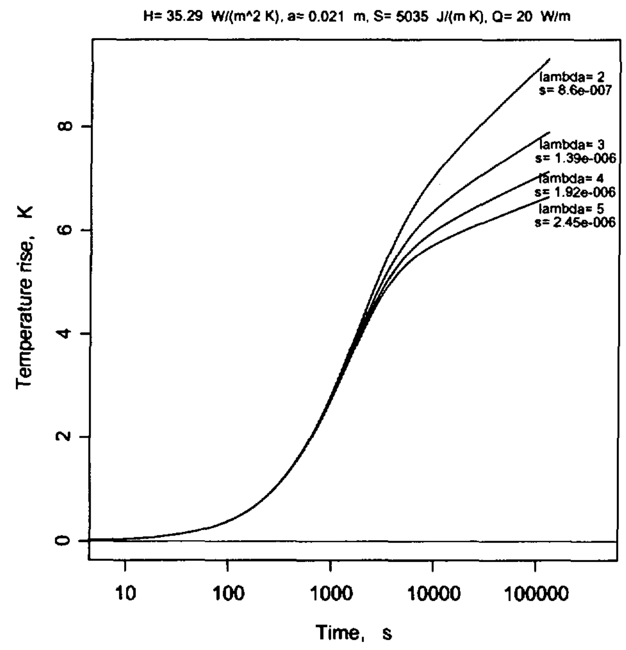

Figure 15. *Theoretical responses of the infinite cylinder probe with varied rock conductivity, 1/thermal contact resistance, H = 35.3.*

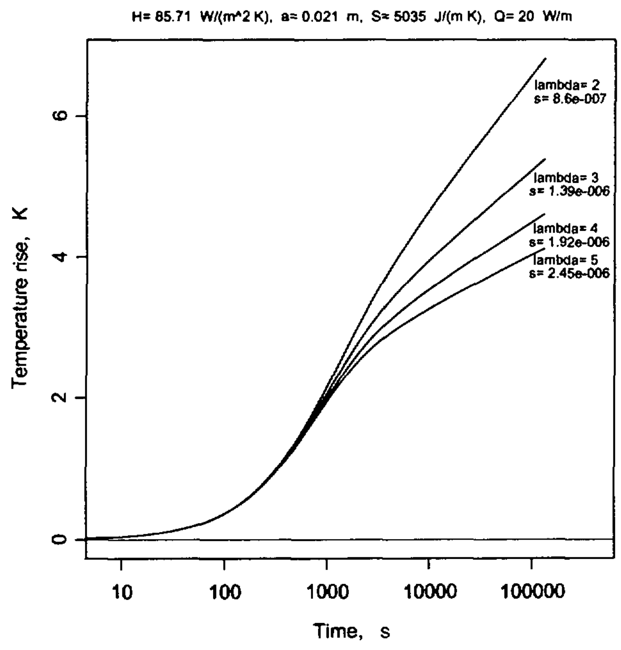

Figure 16. *Theoretical responses of the infinite cylinder probe with varied rock conductivity, 1/thermal contact resistance, H =85.7.*

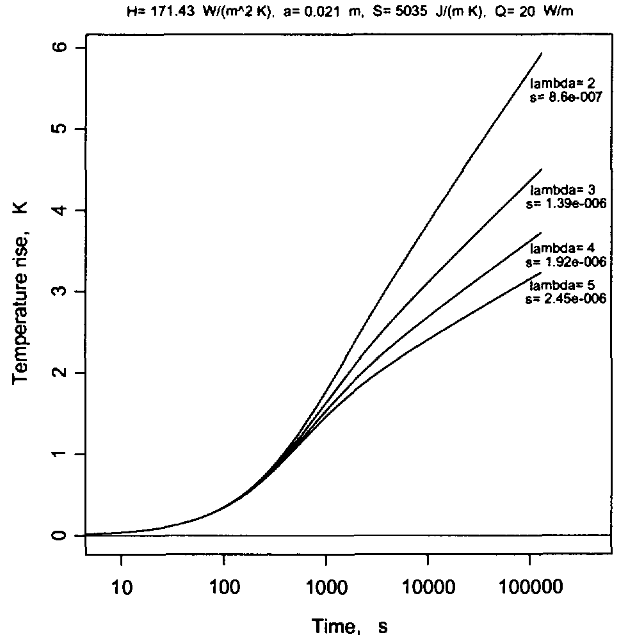

Figure 17. *Theoretical responses of the infinite cylinder probe with varied rock conductivity, 1/thermal contact resistance, H =171.4.*

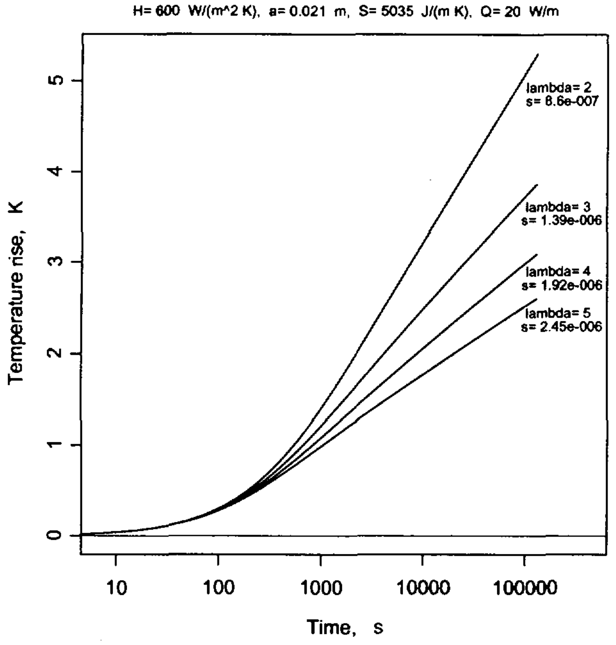

Figure 18. *Theoretical responses of the infinite cylinder probe with varied rock conductivity, 1/thermal contact resistance, H =600.*

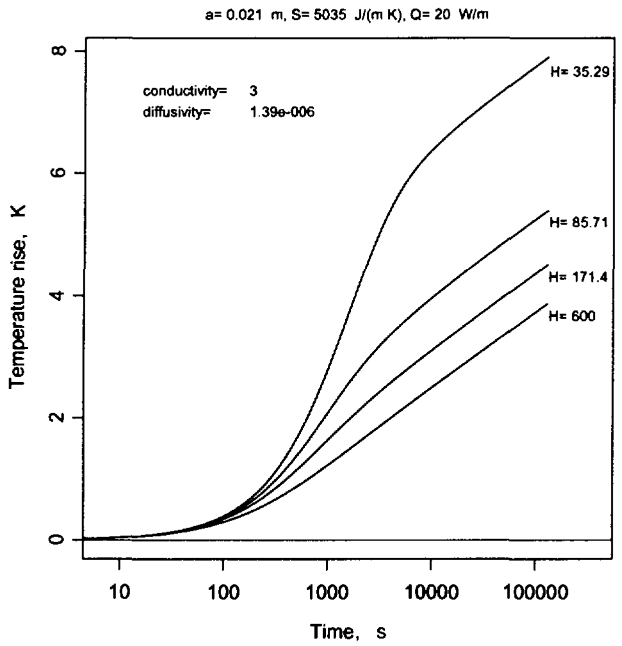

Figure 19. *Theoretical responses of the infinite cylinder probe with varied inverse of thermal contact resistance H. Conductivity is 3.0 W m^{-1} K^{-1}.*

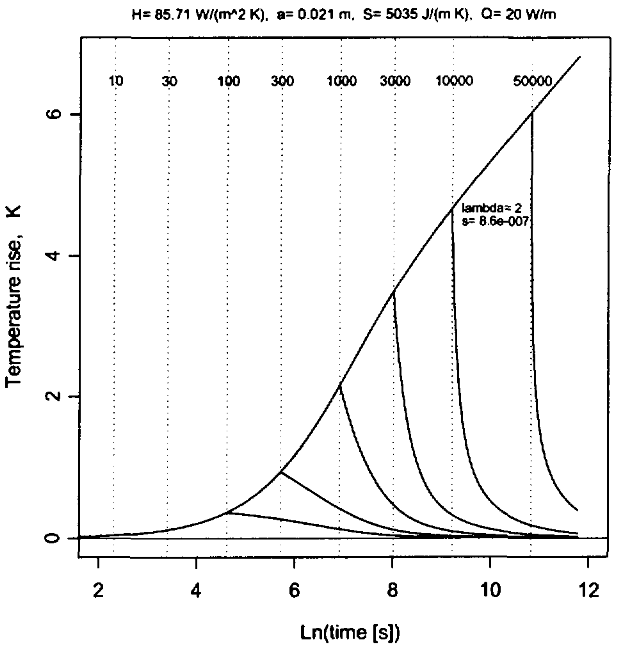

Figure 20. *Theoretical responses of the infinite cylinder probe for a heating pulse. The length of the pulse is varied. Conductivity is 2.0 W m^{-1} K^{-1}. Time axis is logarithmic.*

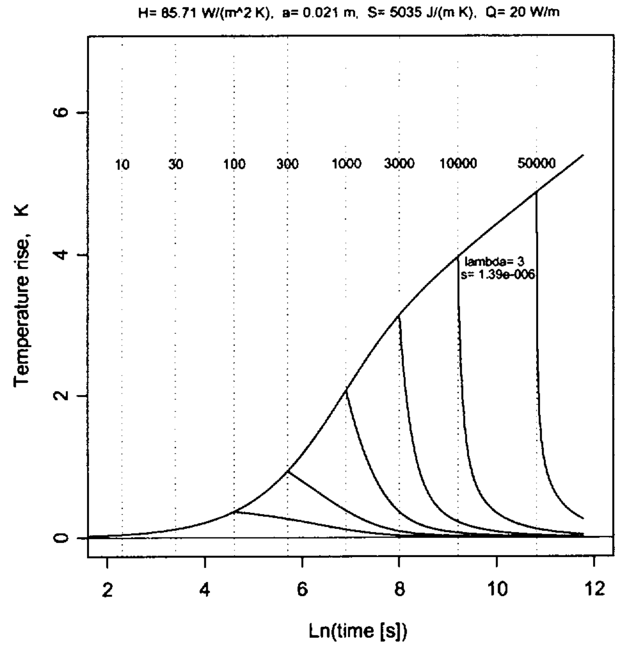

Figure 21. *Theoretical responses of the infinite cylinder probe for a heating pulse. The length of the pulse is varied. Conductivity is 3.0 W m^{-1} K^{-1}. Time axis is logarithmic.*

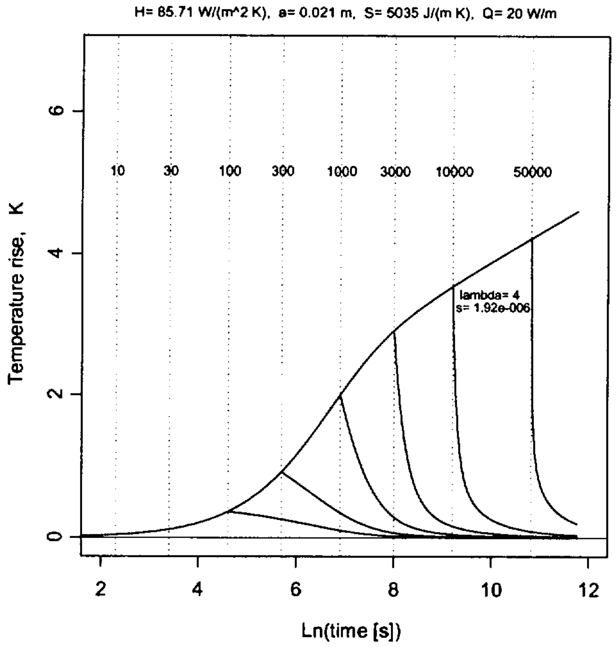

Figure 22. *Theoretical responses of the infinite cylinder probe for a heating pulse. The length of the pulse is varied. Conductivity is 4.0 W m^{-1} K^{-1}. Time axis is logarithmic.*

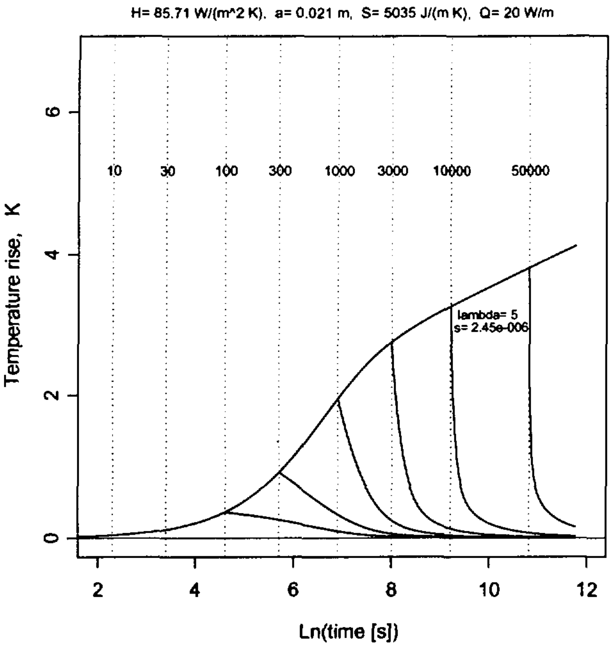

Figure 23. *Theoretical responses of the infinite cylinder probe for a heating pulse. The length of the pulse is varied. Conductivity is 5.0 W m^{-1} K^{-1}. Time axis is logarithmic.*

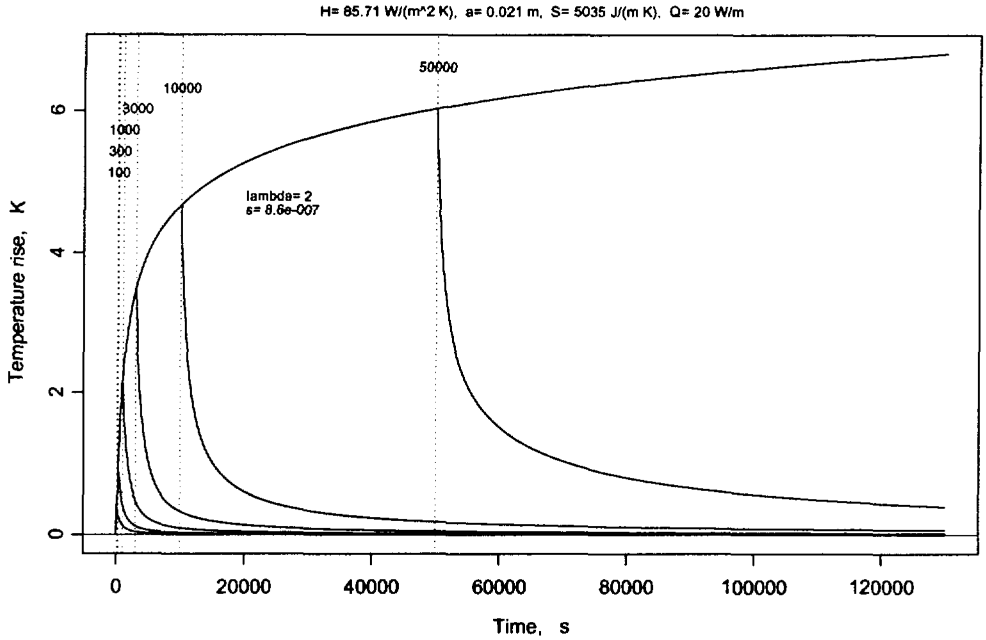

Figure 24. *Theoretical responses of the infinite cylinder probe for a heating pulse. The length of the pulse is varied. Conductivity is 2.0 W m^{-1} K^{-1}. Time axis is linear.*

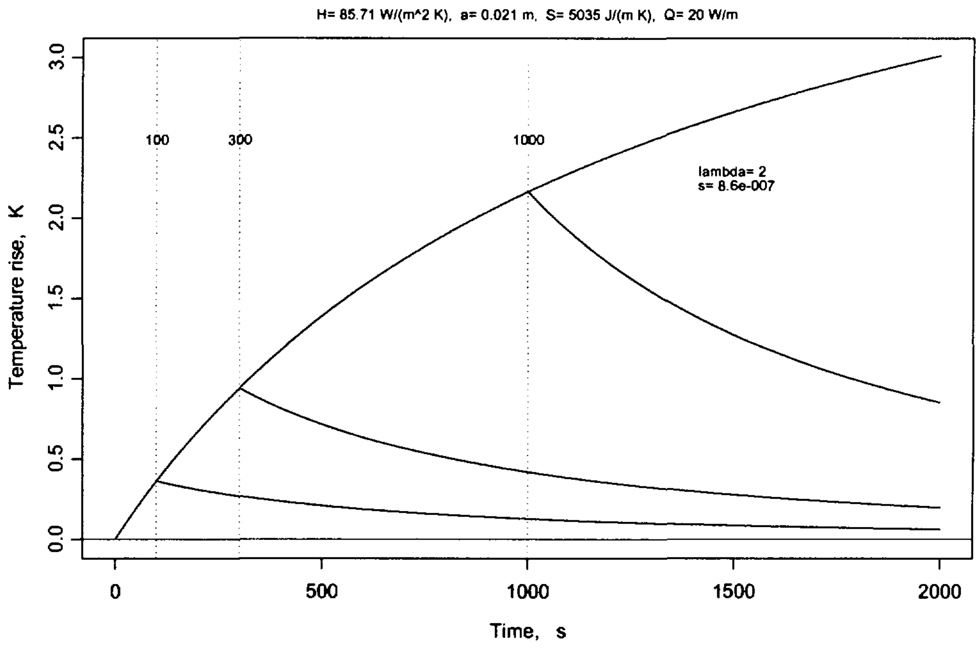

Figure 25. *The same results as in Fig. 24, but in an enlarged view for times 0-2000 s.*

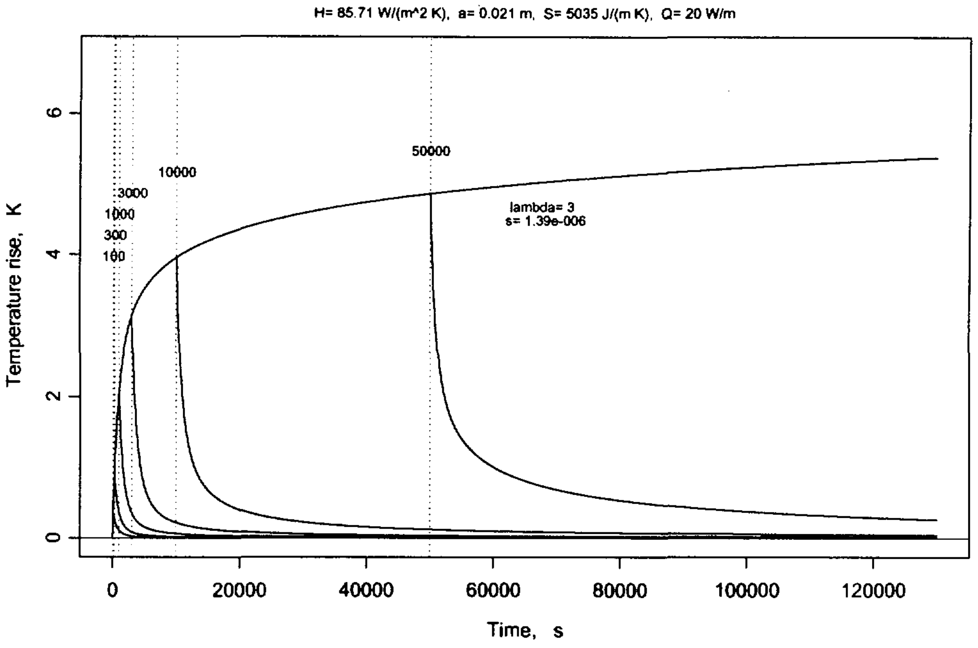

Figure 26. *Theoretical responses of the infinite cylinder probe for a heating pulse. The length of the pulse is varied. Conductivity is 3.0 W m^{-1} K^{-1}. Time axis is linear.*

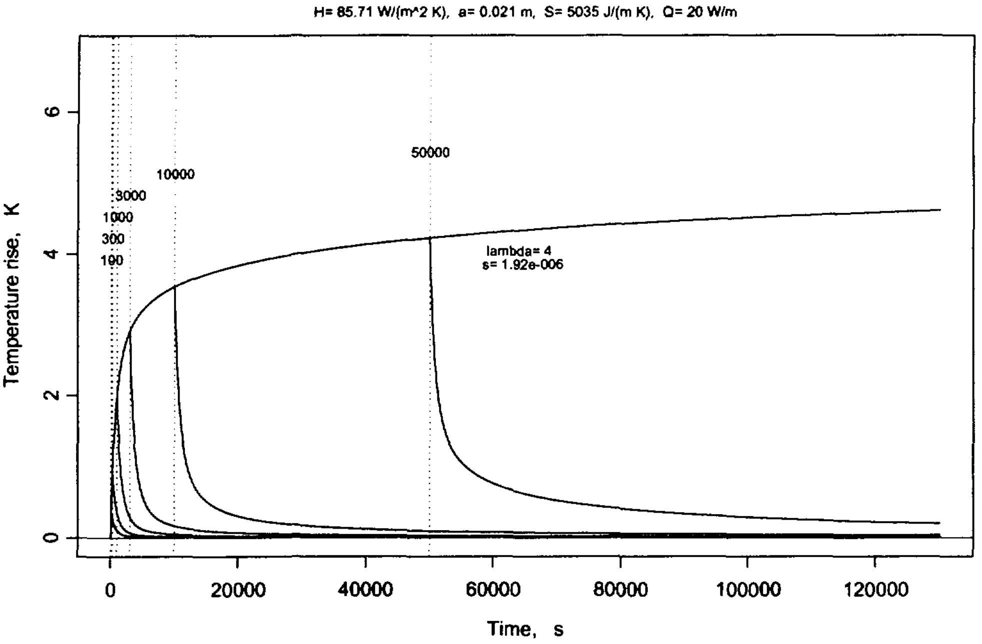

Figure 27. *Theoretical responses of the infinite cylinder probe for a heating pulse. The length of the pulse is varied. Conductivity is 4.0 W m^{-1} K^{-1}. Time axis is linear.*

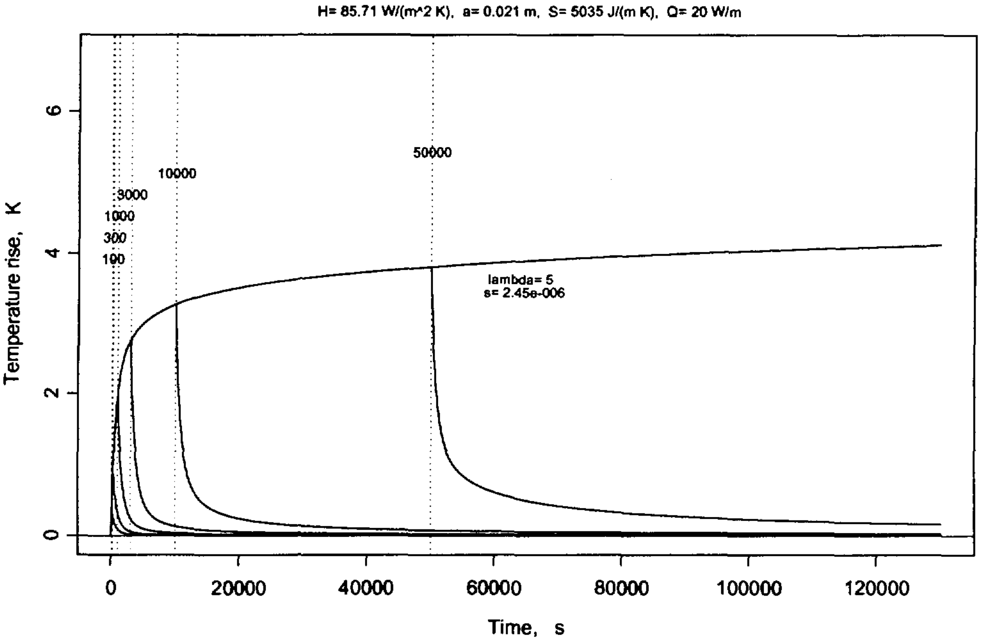

Figure 28. *Theoretical responses of the infinite cylinder probe for a heating pulse. The length of the pulse is varied. Conductivity is 5.0 W m^{-1} K^{-1}. Time axis is linear.*

6.4 Temperature variation in the medium surrounding the hole: Scale of measurement and three-dimensional conduction effects

With the aid of the finite line source solution (eq. 10), the temperature increase outside the measurement hole was modelled for given times 100-50 000 s using continuous heating. No contact resistance was included in these simulations. The results can be used as guide for estimating the effective radius of a measurement, together with estimates calculated from the energy considerations (eq. 2, chapter 5.1).

The temperature decreases very quickly from the hole outward (Figs. 29-35) . After 50 000 s (about 14 hours) of heating the rock temperature is still practically unaffected (temperature increase < 0.1 K) at distances exceeding 0.5 m.

In calculating the temperatures of the surrounding medium, there is not any essential difference between a 2m long line source model and an infinite cylinder source (Figs. 36-37) at distances of 0.1 and 0.3 m. The numerical values are closer than 0.01 K from each other. This suggests that the temperature increase of the external medium can well be approximated with a line source model.

The finite length of the heat source produces axial conduction which produces a deviation of the true probe temperatures from the ideal infinitely long cylinder solution. The finite length of the source is investigated in Figs. 38-39. Temperatures were calculated at a distance of 0.028 m from a 2 m long line source. The situation would correspond to making measurements at the surface of a 56 mm drill hole. The axial 'leak' is indicated by the decreasing temperatures with increasing distance measured along the dimension parallel to the source. In short measurement times the effect is negligible, but becomes increasingly significant at times exceeding 25 000 s, and at 100 000 s (about one day) not even at the central part of the source the temperature is anymore identical to the infinite line source solution in the case of good conductivity. The result suggests that the infinite line (or cylindrical) source solutions are not sufficient for determining thermal properties from experiments of such a long duration. Either the probe must be made longer or a numerical solution for the finite cylinder must be used. However, a first approximation of the correction could be obtained by comparing the solutions for line sources of finite and infinite lengths.

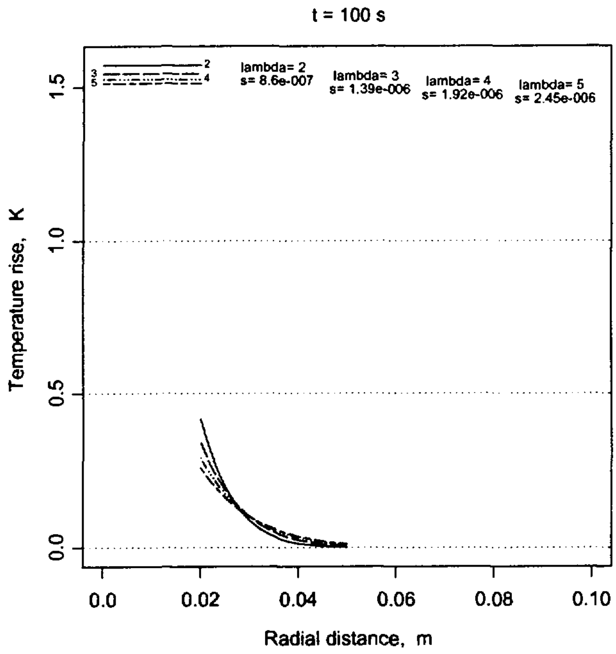

Figure 29. *Temperature increase outside the infinite cylinder probe with continuous heating. Rock conductivity is varied. Time is 100 s, H = 85.7, S = 724.2.*

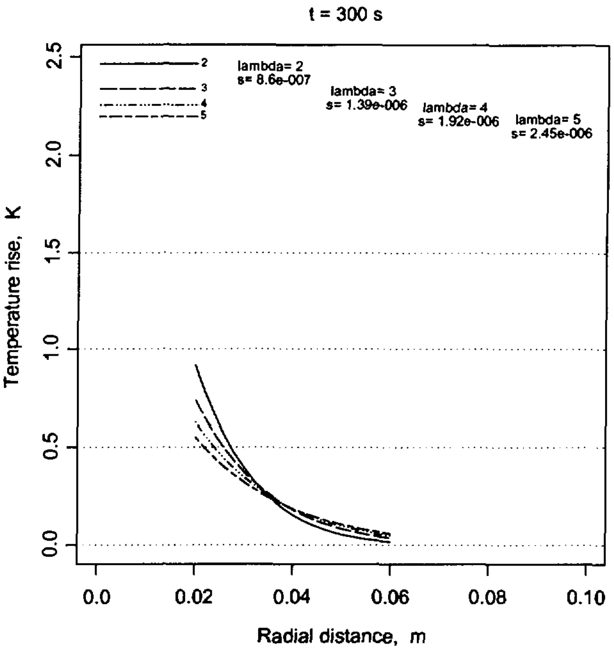

Figure 30. *Temperature increase outside the infinite cylinder probe with continuous heating. Rock conductivity is varied. Time is 300 s, H = 85.7, S = 724.2.*

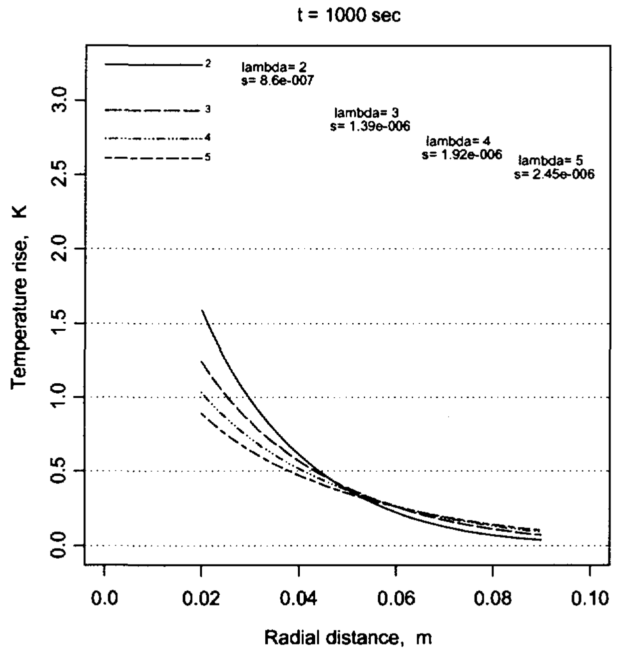

Figure 31. *Temperature increase outside the infinite cylinder probe with continuous heating. Rock conductivity is varied. Time is 1000 s, H = 85.7, S = 724.2.*

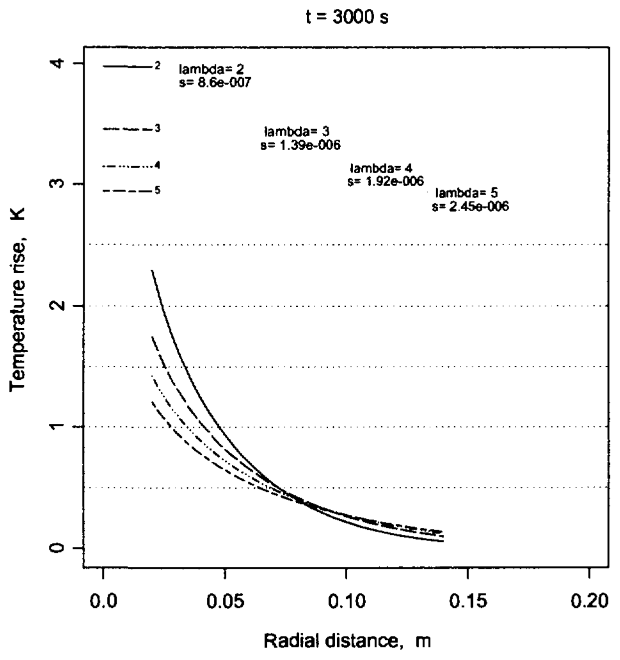

Figure 32. *Temperature increase outside the infinite cylinder probe with continuous heating. Rock conductivity is varied. Time is 3000 s, H = 85.7, S = 724.2.*

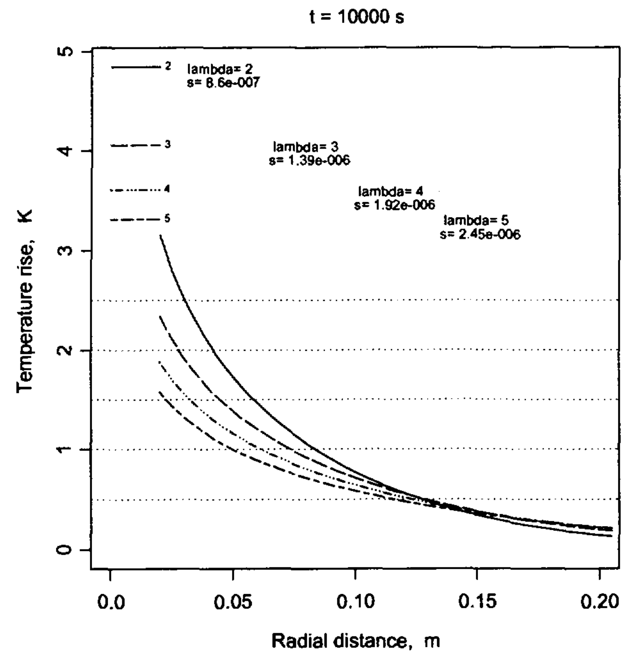

Figure 33. *Temperature increase outside the infinite cylinder probe with continuous heating. Rock conductivity is varied. Time is 10000 s, H = 85.7, S = 724.2.*

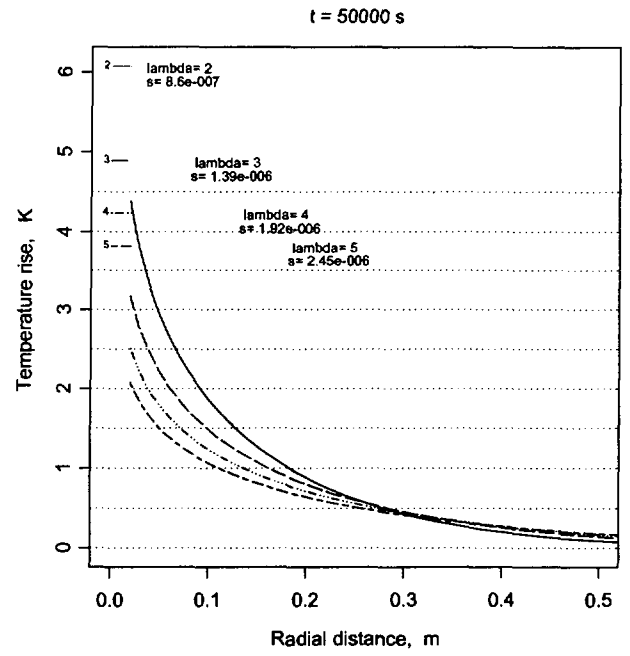

Figure 34. *Temperature increase outside the infinite cylinder probe with continuous heating. Rock conductivity is varied. Time is 50000 s, H = 85.7, S = 724.2.*

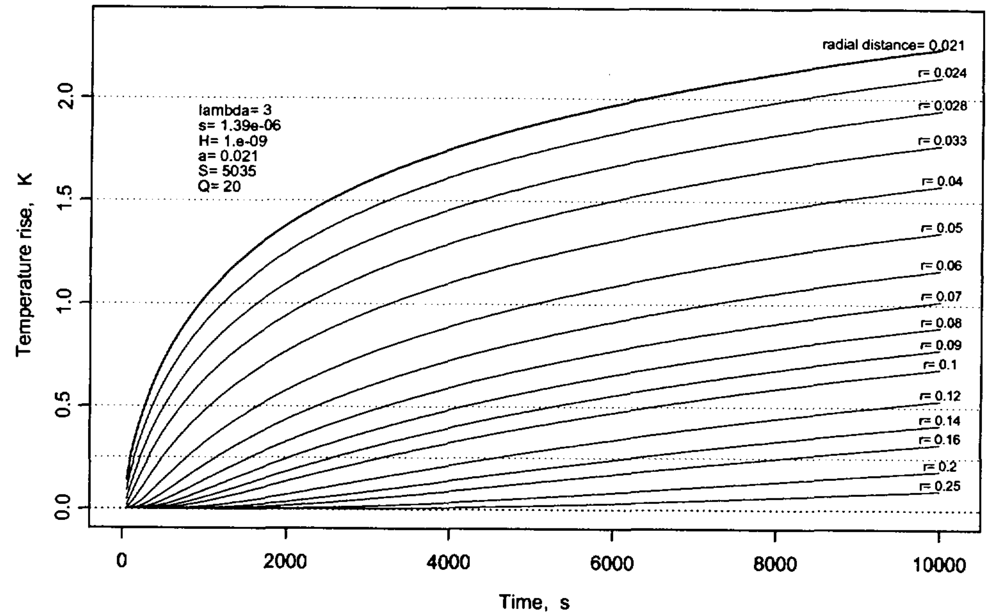

Figure 35. *Temperature increase outside the cylindrical source: distance as the curve parameter.*

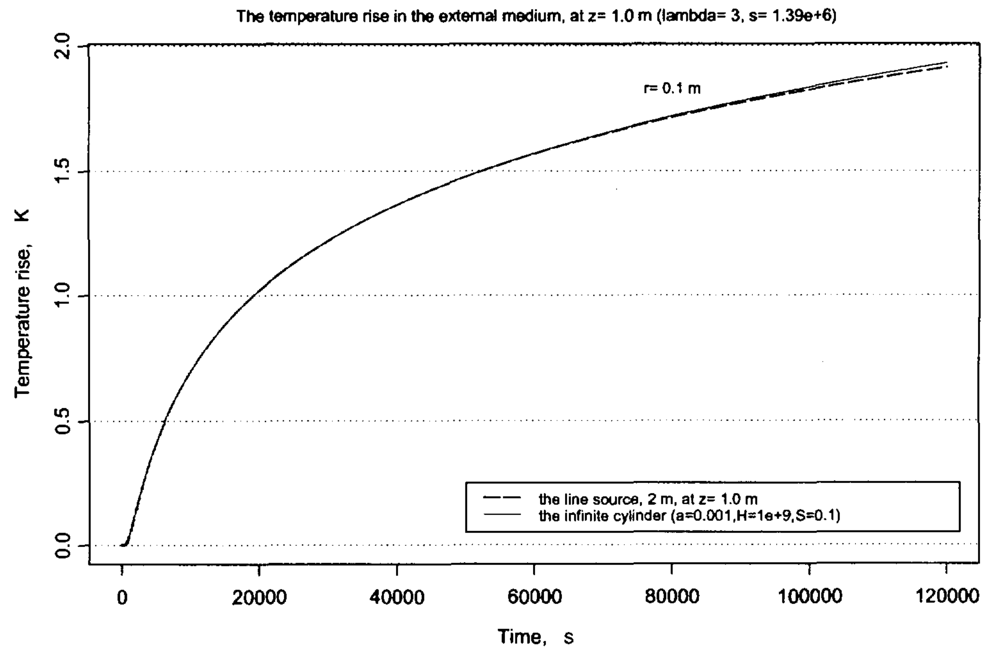

Figure 36. *A comparison between the temperatures calculated at a small distance from the probe with either a finite line source or the infinite cylinder. Distance r = 0.1 m.*

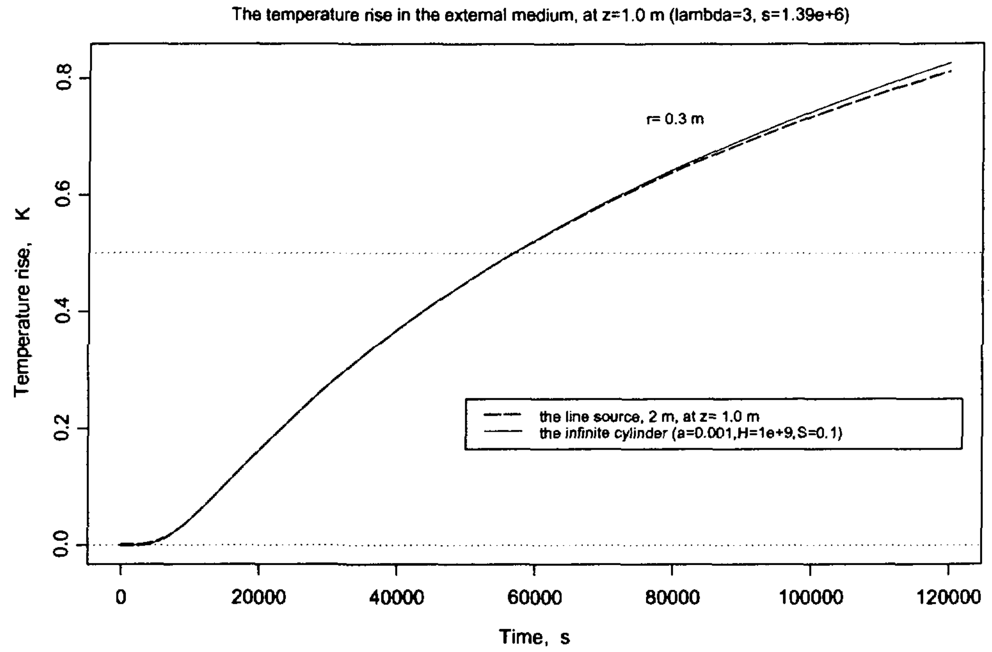

Figure 37. *A comparison between the temperatures calculated at a small distance from the probe with either a finite line source or the infinite cylinder. Distance r = 0.3 m.*

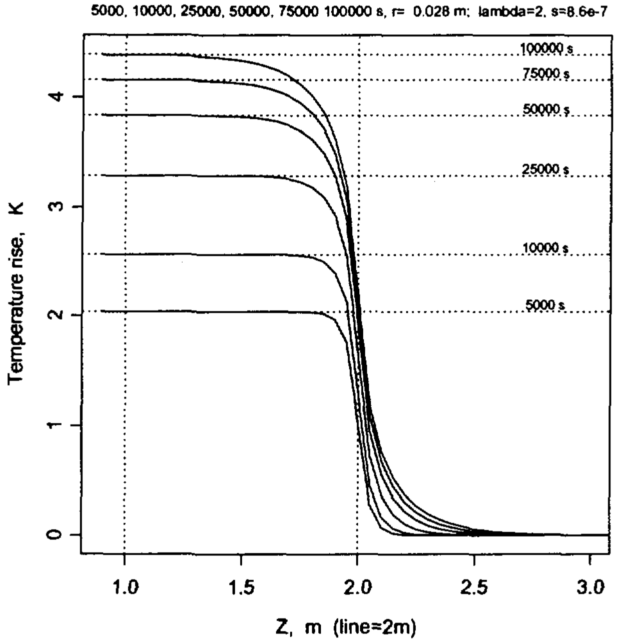

Figure 38. *Differences between the solutions for a finite (2.0 m long) line source and the infinite line source. Distance from the source r = 0.028 m (corresponds to the drill hole wall of a 56 mm hole). Conductivity 2.0 W m^{-1} K^{-1}.*

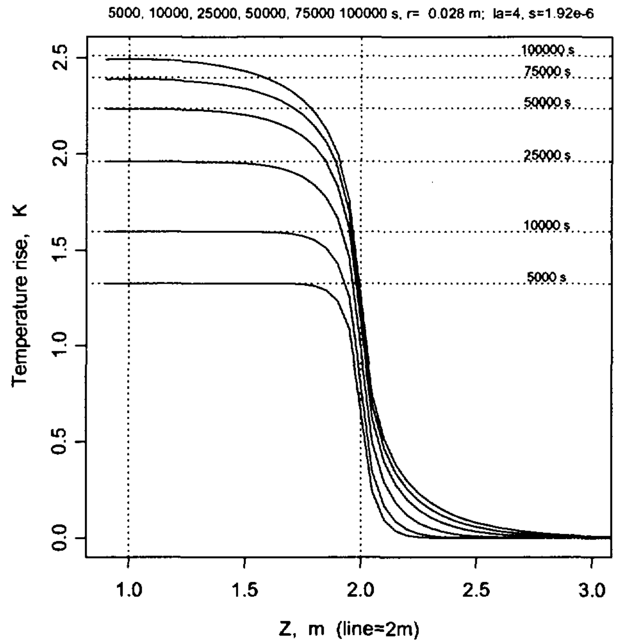

Figure 39. *Differences between the solutions for a finite (2.0 m long) line source and the infinite line source. Distance from the source r = 0.028 m (corresponds to the drill hole wall of a 56 mm hole). Conductivity 4.0 W m^{-1} K^{-1}.*

6.5 Sensitivity of estimated parameters

The resolution and detectability of model parameters were studied in order to find the weak and strong points of single hole measurements. The information content of a data set varies from parameter to parameter, as well as according to the time sequences used for interpretation. Therefore, the importance of measurements (at the time sequence t) relative to the model was analysed. These results contribute to the design of a good heating and measuring practice.

The Jacobian matrix $\partial v(t,p,x)/\partial p$ is also called the sensitivity matrix. It gives useful information of the interpretation task at the time sequence t and at parameter values $(p_i, x_i)^t$. The sensitivity matrix or decompositions of it is usually examined to optimize the measurement system to resolve the model parameters (e.g. Glenn et al, 1973, Pedersen and Hermance, 1986).

The expansion of v in a first-order Taylor's series gives a linearized model for the change of Δv caused by Δp: $\Delta v(t, p, x) = \partial v(t, p, x)/\partial p \times \Delta p$. Following e.g. Pedersen and Hermance (1986) the model parameter will be observable if the shape of the partial derivative curve $\partial v(t, p, x)/\partial p_i$ is sufficiently different from other partial derivative curves of the parameters to be estimated. The model parameter will be detectable if the partial derivative curve has sufficiently large values over the used time period.

The Jacobians $\partial v(\boldsymbol{t}, \boldsymbol{p}, \boldsymbol{x})/\partial p_i \times p_i$ are presented in Fig. 40, where p_i :s are: λ= 3 W/(m°K), s =1.39×10^{-6} m^2/s, H=600 W/(m°K), a=0.021 m, S=5035 J/(m°K) and Q=20 W/m. The heating was ended after 50000 s. If the small chance in a parameter p_i is, for instance, 1%, the chance in the temperature increase is $0.01 \times \partial v(\boldsymbol{t}, \boldsymbol{p}, \boldsymbol{x})/\partial p_i \times p_i$. The shapes of the curves indicate that the correlation of estimated parameters may become a problem. All parameters to be estimated correlate with each other. When the heating continues the correlation between s and H increases but decreases between them and λ. The linear asymptote of $v(t)$ is shown here so that s and H have a constant sensitivity at large heating time. Thus, using only that time period they can not be estimated both simultaneously. The partial derivative curves of s and H differ from each other at times close to start and end of heating. Therefore, these measurement periods are most important for estimating diffusivity s and contact resistance $1/H$.

The effect of small chances in the known probe parameters are shown in Figs. 41-42. The correlations between conductivity λ and power input Q and between the effective probe radius a and s and H are very high.

Monte Carlo simulations were used to study the effect of erroneous measurements and incompletely known model parameters. Using an infinite cylinder model (1) synthetic measurements were generated, and Gaussian noise was added to these responses. These erroneously measured data sets are then interpreted using the "known" model. Different measurement times and pulse lengths were considered.

Results using continuous heating are shown in Figs. 41. Estimated parameters λ, s and H are presented in Fig. 41, when the measuring time is 1000 s, 3000 s and 10000 s. There were 40 simulation runs, the added noise has a standard deviation of 0.1 K. Other parameters are assumed to be known exactly. From these results it is clearly seen that increasing the measuring time improves the accuracy of estimation. Correlations between parameters λ, s and H are high, which means problems at least in short measurement periods.

Correspondingly, results using a heating pulse are given in Fig. 42. They are based on 40 simulation runs with a heating pulse of 3000 s. Results when measurements have been done during the heating period is presented in the upper row, and in lower row the results when measurements have been done after the heating at time period 3005–6005 s. Using the cooling transient the variance of estimated conductivity λ is smaller and the variance of estimated 1/ thermal contact resistance H is larger. The correlations between λ and H and between s and H are smaller during the cooling period.

The results suggest that the diffusivity s will be a much more problematic parameter to *estimate than the conductivity* λ. *This is due to its strong correlation with the contact* resistance, which in a general case is unknown. The error of estimation will be smaller when the thermal contact resistance is lower.

In the previous examples it was assumed that the model was correct. In practice this is a strong assumption. If such an assumption cannot be accepted, and the incorrect model will cause systematic errors to the estimated parameters. A set of results are given in Fig. 43-44 where there are errors in known probe parameters (power, heat capacity), errors in timing accuracy as well as in measured temperature (a trend in temperature measurements).

The results indicate that conductivity is in all cases the best behaving parameter, whereas diffusivity and contact resistance (1/H) are very sensitive to variations in heating power, probe heat capacity, and timing errors. Particularly, a very small trend (linearly increasing error in temperature readings resulting in a 0.04 K error at 100 000 s) in the temperature measurements produces dramatic (up to 50 %) errors in estimated diffusivity and contact resistance (Fig. 44) when the estimation is based on using the whole signal up to 100 000 s. Technically, such a trend may be prevented to be produced by unstable temperature sensors, but such a trend may be encountered in practice if the drill hole temperatures are in a transient state after due to drilling or fluid flow along the hole. Theoretically, the estimation of an erroneous trend together with λ, s and H could be possible when a pulse heating is used. As a result, the bias of diffusivity would be smaller, but of course the variance would be larger. The trend estimate does not correlate with diffusivity.

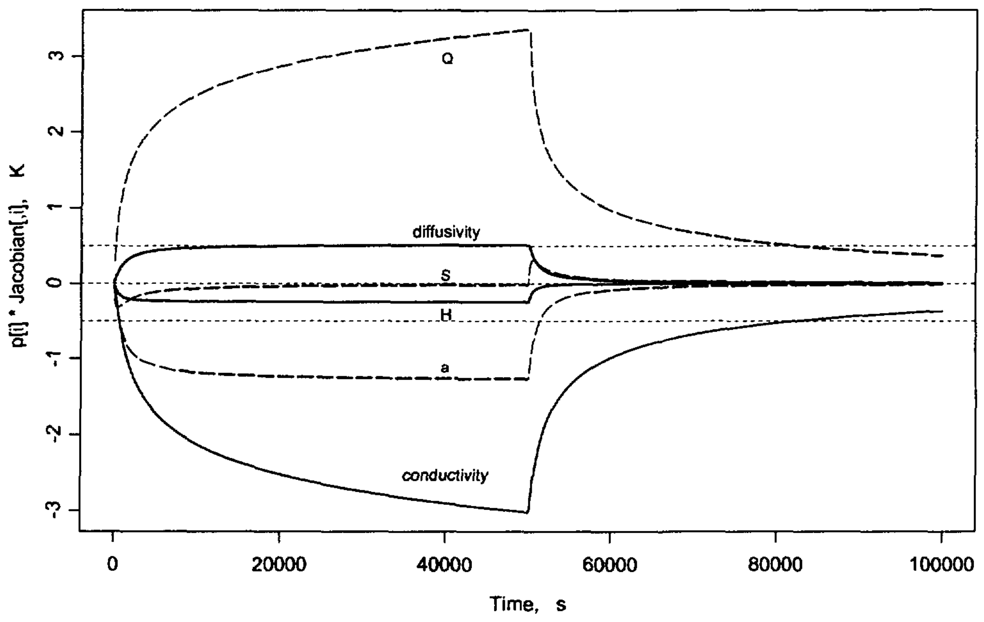

Figure 40. *The Jacobian matrices of inverted parameters as a function of measurement time for a pulse heating of 50 000 s.*

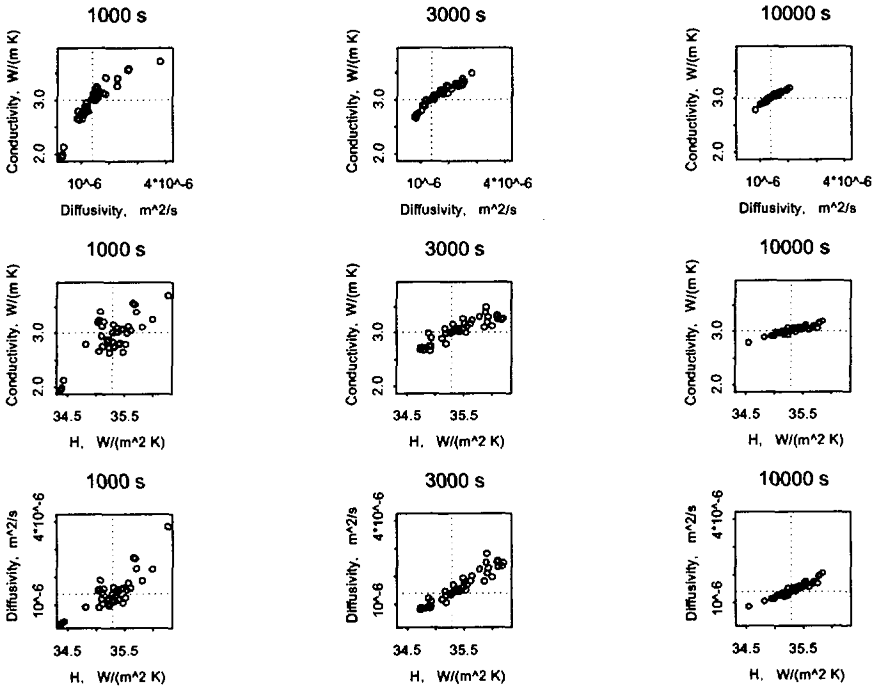

Figure 41. *Cross-plots of inverted parameters with Gaussian noise added in the measured data. Continuous heating assumed. The plots are arranged according to applied time of measurement, 1000, 3000 or 10 000 s.*

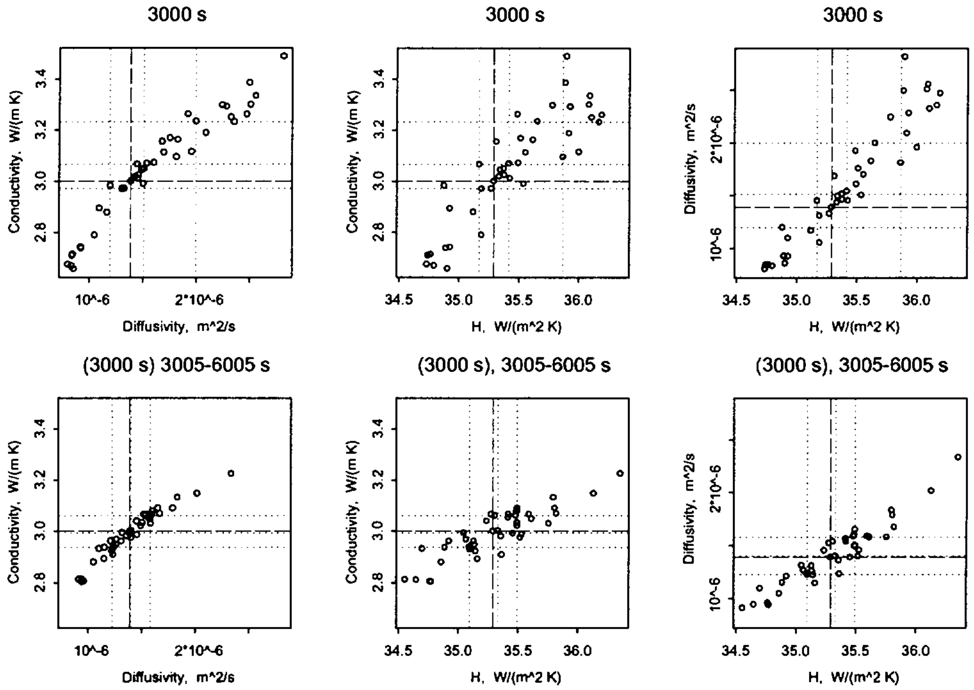

Figure 42. *Cross-plots of inverted parameters with Gaussian noise added in the measured data. Pulse-form heating of 3000 s assumed. The plots are arranged according to applied time of measurement used for inversion, 0-3000 s or 3005-6005 s.*

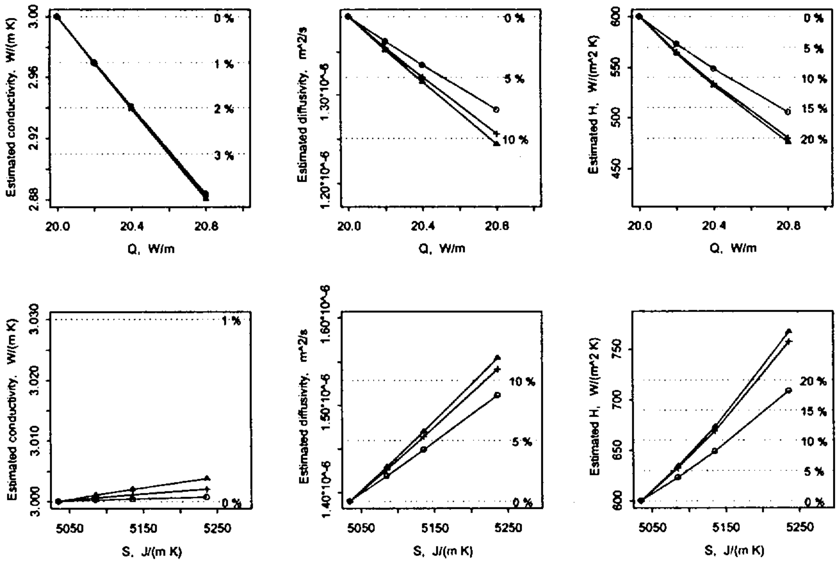

Figure 43. *Sensitivity analysis of inverted parameters (conductivity, diffusivity and inverse of contact resistance) as functions of applied uncertainties in probe heating power and heat capacity. Circles: heating part of a pulse used in the inversion, triangels: cooling part used in the inversion, crosses: both used. Pulse length 50 000 s, measurements up to 100 000 s.*

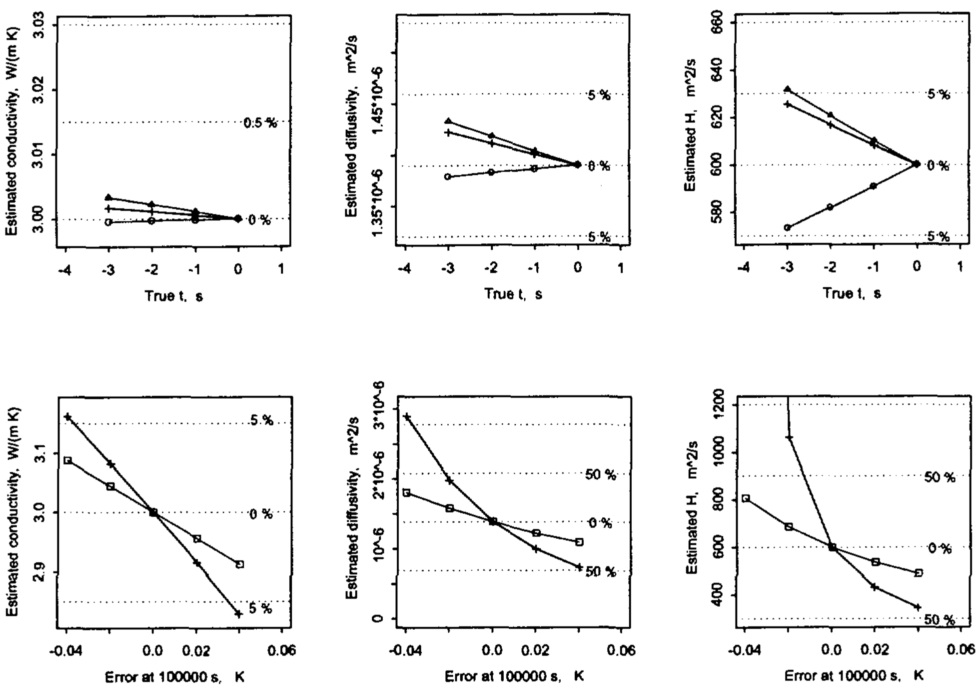

Figure 44. *Sensitivity analysis of inverted parameters (conductivity, diffusivity and inverse of contact resistance) as function of applied uncertainties in the timing accuracy of temperature readings and a trend appearing in temperature measurements. Symbols as in Fig. 43. Pulse length 50 000 s, measurements up to 100 000 s. The results with squares indicate the trend case, but inverted using data only up to 60 000 s.*

6.6 Suggestions for an in situ measurement system

The present theoretical modellings can be used to outline the important factors which should be taken into account in constructing a practical measurement system for single-hole measurements.

Assuming a cylindrical heat source and measurement of its temperature with time, we have to decide on a number of factors: probe material, diameter, length, type of heating signal, as well as duration of experiment, and the applied heating power of the probe.

The applied solutions of heat conduction from a cylindrical heat source are based on the assumption of a infinitely good conductor. The closest practical approximations can be found with metals, such as copper alloys (390 W m^{-1} K^{-1}), aluminium alloys (120-160 W m^{-1} K^{-1}) or brass (120 W m^{-1} K^{-1}).

The diameter of the probe is practically controlled by the limits set by the typical borehole diameter and the minimization of the contact resistance. The aim is to finally construct a probe for 56 mm holes, and therefore, there should be a reasonable clearance between the probe and the borehole wall. Further, the typical drill hole logging tools and cable connectors are often 42 mm in diameter. Therefore we suggest that the probe diameter should be 42 mm which also leaves ample space inside the probe for placing of the measuring and data transportation electronics.

The length of a probe influences the accuracy of the estimated parameters and the effect increases with increasing measuring time. This is due to the failure of the infinite cylinder to approximate the infinitely long heat sources. Theoretical estimates have suggested that the suggested length/diameter ratios should exceed 25 (Blackwell, 1956). In order to reach this value our probe should be about 1 m long. However, as indicated with simulations using an infinite 2 m long line source (Figs 38-39) the leak of heat in the axial direction produces significant deviations from the infinitely long cylinder solutions at measurement times exceeding 30 000 s (about 8 hours). Such a time corresponds to an approximate representative radius of measurement of about 39 cm (eq. 2). Given that the scale of measurement must be made bigger, either the probe must be made longer, or the parameter estimation must be based on a solution for a finite cylinder. Making the probe much longer than 1.5-2 m would not be feasible from the practical point of view, and we suggest that the probe should be 1.5 m long, which would allow practical transportation properties. Temperatures at the centre of such a probe would be good approximations of the infinite cylinder for measurement times as long as about 100 000 s (radius of measurement about 0.7 m). If longer measurement times and larger radii of influence are wanted, a numerical solution for the finite cylinder should be used. This is possible, but not included in the present study.

The heating power of the probe influences directly the measured amplitudes of temperature changes. Technically the power is limited by the logging cables used for input current, and the power very probably should be kept in the range of 5-20 W m^{-1}. Very low powers results in problems with temperature readings due to resolution of the sensors, whereas very high values would result in disturbing convective effects of the drill hole fluid.

Sensitivity analysis of the parameter estimation suggested that conductivity can very probably be reliably estimated but diffusivity is much more problematic. Good diffusivity estimation from single hole measurements would demand careful determination/calibration of probe heat capacity, probe effective radius, and exact quality control of temperature readings.

Theoretically, there is not very much difference in using a continuous heating signal or a pulse signal. However, the sensitivity analysis suggests that a system using pulse heating is slightly more preferable than continuous heating, particularly when diffusivity and contact resistance estimation are considered. Further, if the warming and cooling signals are separated, cooling appears to yield slightly smaller sensitivities for parameter uncertainties.

All forward and inverse solutions are based on the assumption of conductive heat transfer from the probe to the surrounding medium. However, there is a significant risk of convective heat transfer due to natural fluid movement in the hole as well as between the hole and rock. These problems can be eliminated by placing the probe between packers. Two main types of packers have been used in previous applications: either inflatable hydraulic packers (Burkhardt et al., 1995) or simple rubber lamellae (Scroth, 1983) or 'bottle brush' seals (Beck et al., 1971). Inflatable packers would make the measurement system heavier and more complicated to operate, and therefore we suggest more lightweight solutions to be sought for even if they would not be hydraulically perfect in the borehole conditions.

Thus, with the aid of the above modellings we can outline the critical properties of a practical measurement system for 56 mm drill holes. The probe should be about 1.5 m long, with a diameter of 42 mm, and should be operatable in a closed section of a borehole. The heating power should be in the range of 5-20 W m^{-1}. The instrument should be able to collect temperature readings at time intervals ranging from a few seconds to tens of seconds. Generally, a heating pulse should be applied, but the results of an experiment can be utilized in parameter estimation using increasingly longer recordings of temperatures. Thus, the heating section of a pulse signal can be interpreted as a continuous signal experiment with different experiment durations. Thus the scale of investigation increases from one estimate to another, and finally the pulse signal would provide the full data utilization.

The duration of measurements should be extended at least to 100 000 s, which corresponds to a radius of measurement of about 0.7 m. Up to this time the readily available infinite cylinder models yield sufficiently accurate approximations of finite cylinder responses for probe lengths of about 1.5-2 m. In the design of the interpretation sofware, it should be taken into account that measurements concerning longer time periods than 100 000 s, must be modelled with numerical solutions for finite cylinders. With a number of temperature sensors placed along the probe it is also possible to observe the three-dimensional conduction at the probe ends, and with a numerical solution to take full advantage of the measured response along the probe. Due to practical reasons we suggest that the number of temperature sensors should be 5-7.

7 CONCLUSIONS

The thermal transport properties of bedrock *in situ* can be investigated with several methods, such as the cylindrical heat probe method, or indirect estimation methods based on electrical, sonic or compositional borehole loggings, cutting samples and petrophysical relations. Further, a passive method based on transforming a natural temperature gradient log into a thermal conductivity profile could also be developed for the Finnish conditions. Active measurements between boreholes are limited in practice by the slow conduction of heat in rocks, as the propagation of a thermal signal takes already months to a distance of a few metres.

However, the most promising alternative is provided by the cylindrical heat source method for single-hole measurements. This is supported by several factors: (1) the scale of measurement can be controlled by the length of the probe and the time duration of an experiment, (2) a wide range of conductivities can be measured, (3) both conductivity and diffusivity can be measured in a single experiment, and (4) mathematical tools are already available for inverse parameter estimation in the most common measurement situations.

The present theoretical modellings suggest that such a measurement system could give reliable estimates of thermal conductivity within the first metre from the borehole with experiment durations of about one day. However, thermal diffusivity seems to be much more difficult to estimate with high accuracy from such measurements due to correlation with thermal contact resistance between the probe and the borehole wall as well as uncertainties in the probe parameters.

We propose the following factors to be taken as basic parameters in the construction of a practical measurement system: the probe length 1.5-2 m, heating power 5-20 W m^{-1}, temperature recording with 5-7 sensors placed along the probe, and duration of a measurement up to 100 000 s. Assuming these parameters, the interpretation of measurements can be done using the readily available inversion modelling methods based on the solution for the infinitely long cylinder. Experiments with a longer duration can be interpreted using numerical solutions for finite cylinders. A fair accuracy could be achieved by approximating the end losses with the ratios of finite and infinite line solutions.

8 REFERENCES

Allis, R.G. and Garland, G.D., 1976. Geothermal measurments in five small lakes of northwest Ontario. Can. J. Earth Sci., 13, 987-992.

Beck, A.E., 1977. Geothermal measurements in five small lakes of northwest Ontario: Discussion. Can. J. Earth Sci., 14, 332-334.

Beck, A.E. and Shen, P.Y., 1985. Sub-bottom temperature perturbations due to temperature variations at the boundary of inhomogeneous lake or oceanic sediments. Tectonophysics, 121, 11-24.

Beck, A.E., Anglin, F.M. and Sass, J.H., 1971. Analysis of heat flow data - in situ thermal conductivity measurements. Can. J. Earth Sci., 8, 1-19.

Behrens, J., Roters, B. and Villinger, H., 1980. In situ determination of thermal conductivity in cased boreholes. In: A.S. Strub and P. Ungemach (eds.), Advances in European Geothermal Research, Second International seminar on the Results of EC Geothermal Energy Research, March 4-6, 1980, Strasbourg, France. D. Reidel Publ., Dordrecht, pp. 525-534.

Birch, F. and Clark, H., 1940. Thermal conductivity of rocks and its dependence upon temperature and composition. Amer. J. Sci., 238, 529-558 & 613-635.

Blackwell, J.H., 1953. Radial-axial heat flow in regions bounded internally by circular cylinders. Can. J. Phys., 31, 472-479.

Blackwell, J.H., 1954. A transient-flow method for determination of thermal constants of insulating materials in bulk, part I -Theory. J. Appl. Phys., 25, 137-143.

Blackwell, J.H., 1956.The axial-flow error in the thermal conductivity probe. Can. J. Phys., 34, 412-417.

Boggs, P.T., Donaldson, J.R., Byrd, R.H., and Schnabel, R.B., 1989. Algorithm 676 – ODRPACK: Software for weighted orthogonal distance regression: ACM Trans. Math. Software, 15, 348–364.

Bourke, P.J., Hodgkinson, D.P. and Batchelor, A.S.,1978. Thermal effects in disposal of radioactive waste in hard rock. In: Proceedings of the Seminar on in situ Heating Experiments in Geological Formations, Ludvika/Stripa, September 13-15, 1978. OECD Nuclear Energy Agency, pp. 109-117.

Brigaud, F., Vasseur, G. and Caillet, G., 1989. Use of well-log data for predicting detailed in situ thermal conductivity profiles at well sites and estimation of lateral changes in the main sedimentary units at basin scale. In: V. Maury and D. Fourmaintraux (eds.), Proceedings, Rock at Great Depth, Rock Mechanics and Physics at Great Depth, Balkema, Rotterdam, pp. 403-409.

Brigaud, F., Chapman D.S. and Le Douaran, S., 1990. Estimating thermal conductivity in sedimentary basins using lithologic data and geophysical well logs. Am. Assoc. Petrol. Geol. Bull., 74, 1459-1477.

Bullard, E., 1954. The flow of heat through the floor of the Atlantic Ocean. Proc. R. Soc. London, A222, 408-429.

Burkhardt, H., Honarmand, H. and Pribnow, D., 1990. First results of thermal conductivity measurments with a borehole tool for great depths. In: K. Bram, J.K. Draxler, W. Kessels and G. Zoth, Grunlagenforschung und Borlochgeophysik (Bericht 10), Langzeitmess- und Testprogramm in der KTB-Oberpfalz VB. KTB Report 90-6a, Niedersächsiches Landesamt fuer Bodenforschung, Hannover, pp. 245-258.

Burkhardt, H., Honarmand, H. and Pribnow, D., 1995. Test measurments with a new thermal conductivity borehole tool. Tectonophysics, 244, 161-165.

Carslaw, H.S. and Jaeger, J.C., 1959. Conduction of heat in solids. Oxford University Press, Oxford, 510 pp.

Cermak, V. and Rybach, L., 1982. Thermal conductivity and specific heat of minerals and rocks. In: G. Angenheister (editor), Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology, New Series, Group V (Geophysics and Space Research), Vol. 1a (Physical Properties of Rocks), Springer, Berlin, pp. 305-343.

Chan, T. and Jeffrey, J.A., 1983. Scale and water saturation effects for thermal properties of low-porosity rocks. In: Proceedings of the 24th U.S. Symposium on Rock Mechanics, June 20-23, 1983, College Station, Texas, pp. 287-301.

Clauser, C. and Huenges, E., 1995.Thermal conductivity of rocks and minerals. In: T.J. Ahrens (editor), A Handbook of Physical Constants, Rock Physics and Phase Relations, Vol. 3, Americal Geophysical Union, Washington DC, pp. 105-125.

Conaway, J.G. and Beck, A.E., 1977. Fine-scale correlation between temperature gradient logs and lithology. Geophysics, 42, 1401-1410.

Cook, N.G., and Witherspoon, P.A., 1978. In situ experiments in hard rock: their objectives and design. In: Proceedings of the Seminar on in situ Heating Experiments in Geological Formations, Ludvika/Stripa, September 13-15, 1978. OECD Nuclear Energy

Agency, pp. 97-108.

Davis, E. E., 1988. Oceanic heat-flow density. In: R. Haenel, L. Rybach and L. Stegena (eds.), Handbook of Terrestrial Heat-Flow Density Determination, Kluwer, Dordrecht, pp. 223-260.

Drury, M.J. Allen, V.S. and Jessop, A.M., 1984. The measurement of thermal diffusivity of rock cores. Tectonophysics, 103, 321-333.

Glenn, W. E., Ryu, J., Ward, S. H., Peeples, W. J., and Phillips, R. J., 1973. The inversion of vertical magnetic dipole sounding data: Geophysics, 38, 1109–1129.

Haenel, R., 1979. A critical review of heat flow measurements in sea and lake bottom sediments. In : V. Cermak and L. Rybach (editors), Terrestrial Heat Flow in Europe, Springer, Berlin, pp. 49-73.

Haenel, R., Rybach, L. and L. Stegena (editors.), 1988. Handbook of Terrestrial Heat-Flow Density Determination, Kluwer, Dordrecht, 486 pp.

Hocking, G., Williams, J., Boonlualohr, P., Mathews, I. and Mustoe, G., 1981. Numerical modelling of the near surface test facility No. 1 and No. 2 heater tests. In: 22nd U.S. Symposium on Rock Mechanics, Rock Mechanisc from Research to Application, June 28-July 2, 1981, Cambridge, USA. Balkema, Cambridge, USA, pp. 149-155.

Hodgkinson, D.P. and Bourke, P.J., 1978. The far field effects of a radioactive waste repository in hard rock. In: Proceedings of the Seminar on in situ Heating Experiments in Geological Formations, Ludvika/Stripa, September 13-15, 1978. OECD Nuclear Energy Agency, pp. 237-249.

Horai, K., 1971. Thermal conductivity of rock-forming minerals. J. Geophys. Res., 76, 1278-1308.

Hyndman, R.D., Davis E.E. and Wright, J.A., 1979. The measurement of marine geothermal heat flow by a multipenetration probe with digital acoustic telemetry and in situ thermal conductivity. Mar. Geophys. Res., 4, 181-205.

Jaeger, J.C., 1956. Conduction of heat in an infinite region bounded internally by a circular cylinder of a perfect conductor. Austr. J. Phys., 9, 167-179.

Jaeger, J.C., 1958. The measurement of thermal conductivity and diffusivity with cylindrical probes. Trans., Am. Geophys. Union, 39, 708-710.

Jaeger, J.C., 1959. The use of complete temperature-time curves for determination of thermal conductivity with particular reference to rocks. Austr. J. Phys., 12, 203-217.

Jemsek, J. and Von Herzen, R., 1989. Measurement of in situ sediment thermal conductivity: continuous-heating method with outrigged probes. In: J.A. Wright, K.E. Louden and J.R. Moore (editors), CRC Handbook of Seafloor Heat Flow, CRC Press, Boca Raton, Florida, pp. 91-120.

Jolivet, J. and Vasseur, G., 1982. Sur un essai de mesure directe du flux geothermique in situ. Ann. Geophys., 38, 225-239.

Kalinin, V.V., 1983. In situ determination of the coefficient of thermal conductivity of bottom sediments by the cooling-probe method (theory and experiment). Oceanology, 23, 135-138.

Kopietz, J. and Jung, R., 1978. Geothermal in situ experiments in the Asse salt-mine. In: Proceedings of the seminar on in situ heating experiments in geological formations, Ludvika/Stripa, September 13-15, 1978. OECD Nuclear Energy Agency, pp. 45-59.

Kristiansen, J. I., 1982, The transient cylindrical probe method for determination of thermal parameters of earth materials: GeoSkrifter no. 18, Dept. Geology, Aarhus Univ., 154 p.

Kristiansen, J., Saxov, S., Balling, N. and Poulsen, K., 1982. In situ thermal conductivity measurments of Precambrian, Palaeozoic and Mesozoic rocks on Bornholm, Denmark. Geologiska Föreningens i Stockholm Förhandlingar, 104, 49-56.

Kukkonen, I., 1989. Terrestrial heat flow in Finland, the central Fennoscandian Shield. Geological Survey of Finland, Nuclear Waste Disposal Research, Report YST-68, 99 p.

Kukkonen, I. and Lindberg, A., 1995. Thermal conductivity of rocks at the TVO investigation sites Olkiluoto, Romuvaara and Kivetty. Nuclear Waste Commission of Finnish Power Companies, Report YJT-95-08, 29 pp.

Kukkonen, I. and Lindberg, A., 1998. Thermal properties of rocks at the investigation sites: measured and calculated thermal conductivity, specific heat capacity and thermal diffusivity. Posiva Oy, Working Report 98-09e, 29 pp.

Kukkonen, I.T. and Peltoniemi, S., 1998. Relationships between thermal and other petrophysical properties of rocks in Finland. Phys. Chem. Earth, 23, 341-349.

Kuriyagawa, M., Matsunaga, I. and Yamaguchi, T., 1983. An in situ detrmination of the thermal conductivity of granitic rock. In: Fifth International Congress on Rock Mechanics, Melbourne, Australia, Vol. 2, pp. E147-E150.

Langseth, M.G. and Keihm, S.J., 1977. In situ measurements of lunar heat flow. In: J.H. Pomeroy and N.J. Hubbard (eds.), The Soviet-American Conference on Cosmochemistry of the Moon and Planets, June 4-8, 1974, Moscow. NASA Special Publication 370, Part I, pp. 283-293.

Langseth, M.G., Keihm, S.J.,Peters, K., 1976. Revised lunar heat-flow values. In: Proc. of the 7th Lunar Sci. Conf., March 15-19, 1976, Houston, Texas. Pergamon Press, New York, pp. 3143-3171.

Langseth, M.G., Drake, E.M., Nathanson, D., Little, A.D. and Fountain, J.A., 1972. Development of an in situ thermal conductivity measurement for the lunar heat flow experiment. In: Thermal Characteristics of the Moon, Progress in Astronautics and Aeronautics, 28, 169-204.

Lindqvist, G., 1983. Heat flow density measurements in the bottom sediment of some lakes in northern Sweden. Doctoral thesis 1983:30D, Luleå University of Technology, Luleå, 205 p.

Lindqvist, J.G., 1984. Heat flow density measurements in the sediments of three lakes in northern Sweden. Tectonophysics, 103, 121-140.

Lister, C.R.B., 1979. The pulse method of conductivity measurement. Geophys. J. R. astr. Soc., 57, 451-461.

Louden, K.E. and Wright, J.A., 1989. Marine heat flow data: a new compilation of observations and brief review of its analysis. In: J.A. Wright, K.E. Louden and J.R. Moore (editors), CRC Handbook of Seafloor Heat Flow, CRC Press, Boca Raton, Florida, pp. 3-67.

Mussman, G. and Kessels, W., 1980. An in-situ thermal conductivity probe. In: A.S. Strub and P. Ungemach (eds.), Advances in European Geothermal Research, Second International seminar on the Results of EC Geothermal Energy Research, March 4-6, 1980, Strasbourg, France. D. Reidel Publ., Dordrecht, pp. 556-564.

Oelsner, C. and Rösler, R., 1981. Eine Bohrlochsonde zur gleichzeitigen Messung von Wärmestrom und Wärmeleitfähigkeit in situ. Neue Bergbautechnik, 11, 266-268.

Parasnis, D., 1974. Estimates of in situ thermal diffusivity of the ore-bearing rocks in some drillholes in the Skellefte field (N. Sweden) using the annual temperature wave. J. Geophys., 40, 83-95.

Pedersen, J., and Hermance, J. F., 1986. Least squares inversion of one-dimensional magnetotelluric data: an assessment of procedures employed by Brown University: Surveys in Geophysics, 8, 187–231.

Philip, J.R., 1961. The theory of heat flux meters. J. Geophys. Res., 66, 571-579.

Popov, Yu. A., Berezin, V.V., Solov'yev, G.A., Romushkevich, R.A., Korostelev, V.M., Kostyurin, A.A. and Kulikov, I.V., 1987. Thermal conductivity of minerals. Izvestiya, Earth Physics, 23, 245-253.

Pribnow, D. and Sass, J.H., 1995. Determination of thermal conductivity for deep boreholes. J. Geophys. Res., 100, 9981-9994.

Pribnow, D., Williams, C.F. and Burkhardt, H., 1993. Well log-derived estimates of thermal conductivity in crystalline rocks penetrated by the 4-km deep KTB Vorbohrung. Geophys. Res. Lett., 20, 1155-1158.

Raiko, H., 1996. Käytetyn polttoaineen loppusijoituksen lämpötekninen optimointi (Thermal optimization of the final disposal of spent nuclear fuel). Posiva raportti - Posiva Report 96-03, 54 pp. (in Finnish with English abstract).

Rotfuchs, T., 1978. Investigations on the borehole climate in an in situ simulation experiment in the Asse salt mine - a presentation of the concept and preliminary works. In: Proceedings of the seminar on in situ heating experiments in geological formations, Ludvika/Stripa, September 13-15, 1978. OECD Nuclear Energy Agency, pp. 61-70.

Sass, J.H., Kennelly, J.P., Wendt, W.E. Moses, T.H. Jr. and Ziagos, J.P., 1981. In-situ determination of heat flow in unconsolidated sediments. Geophysics, 46, 76-83.

Scroth, G.J., 1983. A new probe for the in situ determination of the heat flow density in shallow cased boreholes. Zbl. Geol. Paläontol., Teil 1, 5-16.

Sundberg, J., 1988. Thermal properties of soils and rocks. Chalmers University of Technology and University of Gothenburg, Department of Geology, Publ. A 57 (dissertation), 47 pp.

Tan, Y. and Ritchie, A.I.M., 1997. In situ determination of thermal conductivity of waste rock dump material. Water, Air and Soil Pollution, 98, 345-359.

Wilhelm, H., 1990. A new approach to the borehole temperature relaxation method. Geohys. J. Int., 103, 469-481.

Williams, C.F. and Anderson, R.N., 1990. Thermophysical properties of the Earth's crust: in situ measurements from continental and ocean drilling. J. Geophys. Res., 95, 9209-9236.

Williams, C.F. Anderson, R.N. and Broglia, C., 1988. In situ investigation of thermal conductivity, heat production, and past hydrothermal circulation in the Cajon Pass scientific drillhole, California. Geophys. Res. Lett., 15, 985-988.

Wright, J.A. and Garland, G.D., 1968. In situ measurement of thermal conductivity in the presence of transverse anisotropy. J. Geophys. Res., 73, 5477-5484.

Xu, H. and Desbrandes, R., 1990. Formation evaluation using in situ measurments of formation thermal properties. SPWLA 31st Annual Logging Symposium, June 24-27, 1990, pp. 1-25.

Yamada, S.E., 1982. A transient technique for in situ thermal property measurements. Int. J. Rock Mech. Min. Sci & Geomech. Abstr., 19, 149-152.

POSIVA REPORTS 1999, situation 1/99

POSIVA 99-01	Measurement of thermal conductivity and diffusivity in situ: Literature survey and theoretical modelling of measurements *Ilmo Kukkonen, Ilkka Suppala* Geological Survey of Finland January 1999 ISBN 951-652-056-1