Numerical evaluation of pressure and temperature effects on thermal conductivity: Implications for crustal geotherms

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RESUMEN

En el presente trabajo se discuten los efectos de la presión y la temperatura sobre la conductividad térmica basados en datos publicados. El problema de transferencia de calor por conducción en estado estacionario, tomando en cuenta la producción de calor y considerando la conductividad térmica como una función de la presión y de la temperatura, satisface una complicada ecuación diferencial no lineal. Aquí se discuten dos soluciones a dicha ecuación: i) una solución analítica utilizando la aproximación de integrales transcendentales y ii) una solución numérica usando un esquema centrado de diferencias finitas. En ambos casos se supone que la producción de calor debida a la presencia de elementos radiogénicos en las rocas satisface un decaimiento exponencial dependiendo de la profundidad.

Con el fin de observar el efecto de la conductividad $\lambda(T,P)$ sobre el campo de temperaturas se resolvió un ejemplo suponiendo una estructura continental de 3 estratos con distintos parámetros geotérmicos hasta una profundidad de 35 km (discontinuidad de Moho) y se consideró un flujo de calor en superficie variando de 50 a 110 mWm^{-2}. Los resultados obtenidos muestran que los efectos de la presión en la conductividad térmica pueden ser despreciados en los estratos superiores; sin embargo para los casos en que el flujo de calor superficial es grande, el efecto se vuelve importante a partir de 5 km de profundidad. En todos los casos el efecto de la temperatura sobre la conductividad térmica muestra variaciones importantes del campo de temperaturas debajo de la discontinuidad de Conrad.

PALABRAS CLAVE: Conductividad térmica, geotermia, estado térmico de la corteza.

ABSTRACT

Pressure and temperature effects on the thermal conductivity of crustal rocks are discussed on the basis of published data. The solution of the steady-state conductive heat equation with pressure-dependent thermal conductivity and heat production leads to a complex non-linear form. Two solutions are discussed: (i) an analytical solution based on an approximation of the transcendental integrals ; (ii) a numerical solution using a finite-difference scheme. In both cases, the heat production due to radiogenic elements is assumed to decay exponentially with depth. An example based on a 3-layer continental structure was solved in order to evaluate the temperature differences at a depth of 35 km (Moho discontinuity). A surface heat flow ranging between 50 and 110 mW/m^2 was assumed. The calculations show that the pressure effect on thermal conductivity can be neglected in the uppermost layers, but for large surface heat flow values, the effect can be important below 5 km.

KEY WORDS: Thermal conductivity, geotherm, thermal state of the crust.

INTRODUCTION

The distribution of temperatures within the crust is of great importance in many geological problems including petroleum maturation, geothermal resources, thermal state of the crust, and mantle heat flow. Near-surface temperature evolution and thermophysical parameters can be directly determined from drillholes, but the extrapolation to greater depths is less accurate. The use of Fourier's equation assuming steady-state conditions requires a knowledge of the thermal properties, *i.e.* thermal conductivity and heat generation as a function of depth. Laboratory measurements and deep seismic information can also be used to constrain these parameters.

The value of thermal conductivity is easily measured in the laboratory. However, thermal conductivity under crust conditions may greatly differ from laboratory measurements. Although the temperature dependence of thermal conductivity is well known (Kappelmeyer and Haenel,

1974), the pressure effect has been generally considered to be negligible. However, experimental data indicate that pressure has a non-negligible positive effect on thermal conductivity (Seipold and Gutzeit, 1980).

In this paper, we investigate the effect of pressure on thermal conductivity and we compare it with temperature dependence. The effect of pressure dependence was quantified on the position of geotherms and at the crust-mantle boundary.

HEAT EQUATION AND CRUSTAL MODELS

There are several tectonic mechanisms that can induce thermal perturbations which modify the thermal field. The variables affecting the thermal field are pressure, temperature, heat generation, heat flow from the mantle, thickness of the crust and duration of the tectonic process. From a knowledge of the thermal field evolution in a given area, the tectonic regime can be inferred.

In the absence of a complete knowledge of the physico-chemical state, equilibrium conditions are often assumed in tectonic processes. In this case, the thermal field and the thermal properties of geological materials must be known with some accuracy.

All materials can store and transport heat. When two points of a solid body are at different temperatures, under steady state conditions heat will be transported by conduction according to Fourier's law (Carslaw and Jaeger, 1959):

$$\phi = -\lambda \, \mathbf{grad} \, T \; , \tag{1}$$

where ϕ is the heat flow (Wm^{-2}), $T(°C)$ is the temperature, and λ is the thermal conductivity (Wm^{-1} °C^{-1}).

When an amount A of heat is produced in the interior of the medium, the energy balance equation takes the form

$$\mathrm{div} \, (\lambda \, \mathbf{grad} \, T) = -A \quad , \tag{2}$$

where A is the volumetric heat production (Wm^{-3}).

Thus a one-dimensional steady state heat transfer problem in an isotropic medium involves the general equations

$$\begin{cases} \dfrac{d\phi}{dz} = A & (3a) \\[2mm] \dfrac{dT}{dz} = \dfrac{\phi}{\lambda} & (3b) \end{cases}$$

where z is the depth (km) assumed to increase downwards, and A and λ depend on the physico-chemical parameters of the medium.

The application of the heat equation to crustal models is possible under certain assumptions. At the scale of observation, the crust must be in equilibrium with the surrounding media. The erosion at the surface should be negligible, and the mantle flow must be considered constant and of regional extent (Nielsen and Balling, 1985).

The crust is assumed to be composed of N horizontal layers of constant thermal properties and varying rules. The lithology and the thermal properties of each layer are supposed to be known. The layers are assumed to be in perfect thermal contact between each other, and heat transfer takes place only by thermal conduction.

Boundary conditions

The integration constants of Eq. (3) are given by the boundary conditions, *e.g.* the values of heat flow and temperature at boundaries in the crust. The boundary conditions are given at the surface; the conditions at the mantle-crust interface are unknown.

Surface temperatures are greatly influenced by atmospheric conditions. However the thickness of the interface is only a few meters wide (Courtillot and Francheteau, 1976). A mean temperature ranging between 5° to 10°C can be assumed in Europe (Royer and Danis, 1988).

Surface heat flow has been measured in a large variety of geological settings all around the world. It varies from 40-50 mWm^{-2} in old Precambrian platforms, but it can exceed 100 mWm^{-2} in recent granitic crust (Vosges massif, Royer and Danis 1988; French Massif Central, Royer and Danis, 1987, Vasseur, 1982).

Heat generation

Heat generation within the crust is related to the decay of radiogenic elements, particularly ^{238}U, ^{235}U, ^{232}Th and ^{40}K. Because those elements are incompatible, their distribution depends on the fractionation occurring during the formation of the crust. Radiogenic elements are concentrated in the upper crust and their concentration decreases with depth.

Another aspect influencing rock composition is the time of residence of the radiogenic elements. The disintegration reactions are responsible for the disappearance of reactive cores and for the decrease of the radiogenic content. Thus the heat due to radiogenic elements in an old crust is expected to be smaller that in a younger crust.

Seismic velocity profiles can be used to determine heat production with depth (Rybach and Buntebarth, 1984). Different distribution models with depth have been proposed (linear, exponential, hyperbolic, and others) (Cermák et al., 1991). The exponential model (Lachenbruch, 1970) is currently accepted:

$$A(z) = A_o \exp\left(-\frac{z - z_o}{D}\right) \; , \tag{4}$$

where D is a parameter with the dimension of a length, A_o is the surface heat generation and z_o the reference depth (generally $z_o = 0$). The D parameter is taken to represent the vertical distribution of radiogenic elements. Thus, the state of differentiation of the crust is of great importance. According to Cermák et al. (1991), the D value is about 10-15 km in Hercynian terrains and more than 15 km in old Precambrian platforms. The surface heat generation A_o varies from 0.5 μWm^{-3} for Precambrian units to 3 μWm^{-3} in Phanerozoic terrains, though it may locally exceed this value (Royer and Danis, 1988).

Thermal conductivity

Thermal conductivity characterizes the heat transport in solids. Conduction of heat in solids takes place by thermal vibrations of the mineral lattice and by radiative transfer. At low temperatures, the main heat transport process is by phonons produced by lattice conductivity, *i.e*, the vibrations of atoms around their equilibrium position in the crystal lattice (Courtillot and Francheteau,1976). In this case, thermal conductivity decreases with temperature as $1/T$. At higher temperatures, energy transport occurs by photons as T^3 (radiative conductivity; MacPherson and Schloessin, 1982). Classically, conductivity is considered as the sum of lattice and radiative conductivities even though radiative transfer does not play a major role because

of the opacity of most common minerals (Poirier, 1991). Besides, for the range of temperatures in the crust, radiative conductivity can be neglected (Birch and Clark, 1940).

Temperature effect on thermal conductivity

Investigations of single mineral properties show that thermal conductivity varies from 1.5 Wm^{-1}°C^{-1} in plagioclases to more than 5.5 Wm^{-1}°C^{-1} in some pyroxenes and in halite and more than 7.7 Wm^{-1}°C^{-1} in quartz (Horai, 1971). However, thermal conductivity in minerals generally depends on the crystallographic orientation and is thus a tensor of order 3. Modifications of the crystallographic form (polymorphism), for instance the α/β quartz transition, can cause drastic changes in thermal conductivity.

Thermal conductivity of rocks depends on mineralogical composition and structure. Rocks with a high feldspar content have a small conductivity (Birch and Clark, 1940). In acid rocks, thermal conductivity depends on quartz content (Koutsikos, 1985).

Anisotropy in rocks is produced by preferential orientations of minerals. It is particularly evident in sedimentary and metamorphic rocks (schists and gneisses). In some cases, the thermal conductivity of granitic rocks can be taken as isotropic because of the random orientation of rock-forming minerals (Flores, 1992).

The thermal conductivity is taken to vary as the inverse of a linear function of temperature (Carslaw and Jaeger, 1959):

$$\lambda(T) = \lambda^{T_o} \frac{1}{1 + b[T - T_o]} \qquad (5)$$

where λ^{T_o} is the thermal conductivity measured at T_o and b is a material constant generally comprised between 5×10^{-4} and 10^{-3} °C^{-1} (Royer and Danis, 1988), or taken to be equal to 1.5×10^{-3} °C^{-1} (Chapman, 1986). For rocks with a high quartz content the α/β quartz transition has a detectable though very small effect on bulk conductivity.

Figure 1 shows the evolution of thermal conductivity for typical rocks in the temperature range observed in the crust (0 to 600°C). Thermal conductivities always decrease with increasing temperature. Values of *b* ranging from 5×10^{-4} to 29×10^{-4}°C^{-1} have been reported.

Pressure effect on thermal conductivity

Because thermal conductivity reflects the ability of atoms to vibrate around their equilibrium position, pressure is expected to have some influence on thermal properties. The higher the pressure, the shorter is the interatomic distance and the higher the ability of atoms to transfer energy to their neighbours. Hence thermal conductivity is expected to increase with pressure.

However, only few data are available on the thermal conductivity pressure dependence. Experimental results in crystalline and sedimentary rocks show a rapid initial in-

crease which then levels off (Figure 2). The initial rapid increase is lacking for some rocks, *e.g.* charnockite (Seipold and Gutzeit, 1980).
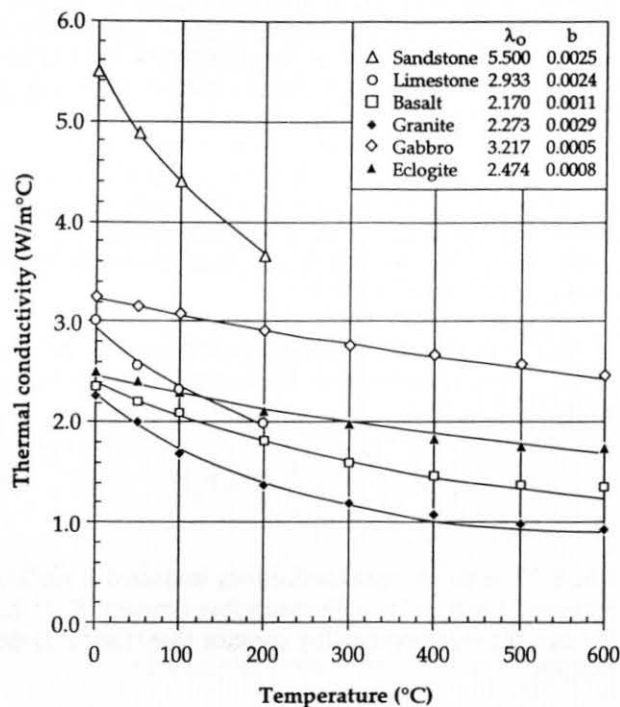

Fig. 1. Thermal conductivity decrease with temperature as $1/T$. Experimental values for some common types of rocks are fitted using λ_o and b in Eq. (5). Data from Kappelmeyer and Haenel (1974).
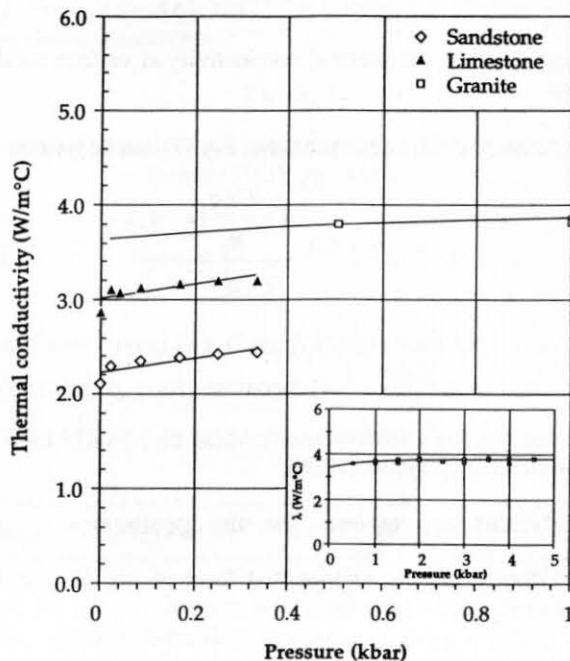

Fig. 2. Thermal conductivity increase with depth. Experimental values to 1 kbar for some common kinds of rocks as reported for some sedimentary rocks (Kappelmeyer and Haenel, 1974) and granite (Seipold, 1992). The inset box shows data for the granite sample to 5 kbar (Seipold, 1992).

The rapid increase of thermal conductivity at low pressures is attributed to the closing of pores and cracks (Walsh and Decker, 1966; Seipold and Gutzeit, 1980). In crystalline rocks, this increase is observed up to 1 kbar. It is mainly due to closing cracks and never exceeds one percent. Porosity of Casco granite, Maine, is 0.004 (Brace, 1965). A similar behaviour is found for sedimentary rocks (Kappelmeyer and Haenel, 1974), but the initial increase is only observed over the first 50 bars.

At higher pressures (>1 kbar for granite and >50 bars for sedimentary rocks), thermal conductivity slowly increases with pressure, and the pressure dependence in most cases can be approximated by a straight line (Seipold and Gutzeit, 1980; Seipold, 1992).

The dependence of thermal conductivity λ on P is given by the linear relation (Guéguen and Palciauskas, 1992):

$$\lambda(P) = \lambda^{P_o}\left(1 + \frac{C}{K_s}[P - P_o]\right) \quad (6)$$

where λ^{P_o} is the thermal conductivity measured at surface pressure (1 atm), C is a dimensionless constant, K_s is the iso-entropic incompressibility constant (bar^{-1}) and P is the pressure.

Combining Eq. (5) and (6) leads to (Chapman, 1986):

$$\lambda(T,P) = \lambda^{T_o,P_o} \frac{1 + \dfrac{C}{K_s}[P - P_o]}{1 + b[T - T_o]} \quad (7)$$

where λ^{T_o,P_o} is the thermal conductivity at surface conditions.

Assuming lithostatic pressure, Eq. (7) can be written

$$\lambda(T,z) = \lambda^{T_o,z_o} \frac{1 + \dfrac{C\rho g}{K_s}[z - z_o]}{1 + b[T - T_o]} \quad (8)$$

where ρ is the rock density (kgm^{-3}), g is gravity (ms^{-2}) and z is depth (m). $\frac{C\rho g}{K_s} = C$ is a constant for a given geological formation; a representative value of 1.5×10^{-4} km^{-1} is proposed by Chapman (1986).

Analytical expressions for the geotherms

Considering the exponential form of Eq. (4) for the heat production, the heat flow is derived by integration of Eq. (3a). For a layer whose top is situated at depth z_1, the heat flow at a depth $z > z_1$ is given by:

$$\phi(z) = A_o D\left[\exp\left(-\frac{z - z_o}{D}\right) - \exp\left(-\frac{z_1 - z_o}{D}\right)\right] + \phi(z_1). \quad (9)$$

Using Eq. (3b), (5) and (7), the temperature distribution as a function of depth is calculated from

$$\frac{dT}{dz} = \frac{\phi(z)}{\lambda(T,z)} = \frac{\phi(z)(1 + b(T - T_o))}{\lambda_o(1 + c(z - z_o))} \quad , \quad (10)$$

which leads to

$$\int_{T_1}^{T} \frac{1}{(1 + b(\tau - T_o))} d\tau = \frac{1}{\lambda_o} \int_{z_1}^{z} \frac{\phi(\zeta)}{1 + c(\zeta - z_o)} d\zeta \quad (11)$$

The mathematical form of the temperature distribution $T(z)$ depends on $\lambda(T,z)$. Three cases of interest are discussed (Table 1):

(A): λ is assumed to be constant (b=c=0). Here $T_A(z)$ is the sum of an exponential function and a linear function of z.

(B): λ depends only on temperature (b≠0; c=0). The solution of Eq. (10) shows that the temperature $T_B(z)$ is an exponential function of $T_A(z)$.

(C): combined dependence upon temperature and depth (b≠0; c≠0), which leads to the following expression:

$$I(z_1, z) = \int_{z_1}^{z} \frac{\exp\left(-\dfrac{\zeta - z_o}{D}\right)}{1 + c(\zeta - z_o)} d\zeta \quad (12)$$

which is a transcendental integral.

We use two methods in order to solve this last case. The first method is based on the iterative solution of Eq. (3) using a finite difference scheme. The crust is divided into a number of sub-layers of constant thickness $\Delta z = z_i - z_{i+1}$. A 100 meter interval was chosen. In each layer, the bottom temperature T_{i+1} was calculated from the top temperature T_i assuming constant thermal conductivity and heat production (Nielsen and Balling, 1985; Chapman, 1986). For a layer Δz the temperature T_{i+1} may be expressed by

$$T_{i+1} = T_i + \frac{\overline{F}_{i/i+1}}{\lambda_i} \Delta z - \frac{\overline{A}_{i/i+1}}{2\lambda_i} \Delta z^2 \quad (13)$$

where $\overline{A}_{i/i+1}$ is the mean heat production taken as the average of the heat production A_i in the upper layer and the heat production A_{i+1} in the lower layer, estimated from Eq. (4). Similarly, $\overline{F}_{i/i+1}$ is the mean heat flow as computed from F_i, the heat flow at the base of the layer, and F_{i+1}, the heat flow at the top, estimated from Eq. (8). Thermal conductivity λ_i is calculated from T_i and z_i using Eq. (8).

The second method uses an approximation of the transcendental integral (12). If we define

$$s = \frac{1 + c(\zeta - z_o)}{cD} \quad , \quad (14)$$

Table 1

Analytical expressions of the geotherm when the thermal conductivity depends on temperature and pressure. T_o and z_o are the reference temperature and depth at which λ_o is applied, while T_1 and z_1 are the temperature and depth at the upper boundary of the considered layer.

Thermal conductivity model	Solution
$\lambda = \lambda_o$	$T_A(z) = -\dfrac{A_o D^2}{\lambda_o}\exp\left(-\dfrac{z-z_o}{D}\right) + \dfrac{\phi(z_1) - A_o D \exp\left(\dfrac{z_1-z_o}{D}\right)}{\lambda_o}(z-z_1) + \dfrac{A_o D^2}{\lambda_o}\exp\left(-\dfrac{z-z_o}{D}\right) + T_1 = F(z) + T_1$
$\lambda = \lambda_o \dfrac{1}{1+b(T-T_o)}$	$T_B(z) = \dfrac{1+b(T_1-T_o)}{b}\exp(bF(z)) - \dfrac{1}{b} + T_o$
$\lambda = \lambda_o \dfrac{1+c(z-z_o)}{1+b(T-T_o)}$	$T_C(z) = \dfrac{1+b(T_1-T_o)}{b}\exp\left[\dfrac{b}{c\lambda_o}G(z)\right] - \dfrac{1}{b} + T_o$ with (*) $G(z) = A_o \exp\left(\dfrac{1}{cD}\right)\left[E1\left(\dfrac{1+c(z_1-z_o)}{cD}\right) - E1\left(\dfrac{1+c(z-z_o)}{cD}\right)\right] + \left(\phi(z_1) - A_o D \exp\left(-\dfrac{z_1-z_o}{D}\right)\right) \text{Log}\dfrac{1+c(z-z_o)}{1+c(z_1-z_o)}$

(*) for definition of the E1 function; see text

then $I(z_1, z)$ can be expressed analytically as

$$I(z_1, z) = \frac{1}{c}\exp\left(\frac{1}{cD}\right)\left[\int_{s_o}^{+\infty}\frac{\exp(-s)}{s}ds - \int_{s_1}^{+\infty}\frac{\exp(-s)}{s}ds\right] \quad . \quad (15)$$

The function $\int_x^{+\infty}\frac{\exp(-s)}{s}ds$ is the exponential integral $E_1(x)$ which can be approximated by the functions given in Table 2 (Abramowitz and Stegun, 1970, pp. 228-231). The expression of $T_C(z)$ is given in Table 1.

APPLICATION TO CRUSTAL MODELS

A crustal model was developed to estimate the influence of pressure and temperature on thermal conductivity. This model is composed from top to bottom of a 3 km thick sedimentary layer, a 13 km granitic basement, and a granulitic lower crust reaching down to the Moho at 35 km (Cermák, 1989).

The thermophysical properties, based on average values for continents, are given in Table 3. The heat production of the lower crust was taken as a constant since it is very low relative to the other layers (Chapman, 1986). Surface heat flow values ranging from 50 to 110 mWm^{-2} were assumed

and three models of thermal conductivity dependence were compared: following Eq. (5), following Eq. (7) and with a constant conductivity.

Table 2

Approximation of the E1 function (after Abramowitz and Stegun, 1970, pp. 228-231)

Validity	$0 < s < 1$	$s > 1$	
E1(s)	$\displaystyle\sum_{i=0}^{5} a_i s^i - \ln(s) + \varepsilon(s)$	$\dfrac{1}{s\exp(s)}\dfrac{\displaystyle\sum_{i=0}^{4} a_i s^i}{\displaystyle\sum_{i=0}^{4} b_i s^i} + \varepsilon(s)$	
error	$\varepsilon I(s) < 2\ 10^{-7}$	$\varepsilon I(s) < 2\ 10^{-8}$	
i	a_i	a_i	b_i
0	- 0.57721 566	1	1
1	0.99999 193	8.57332	9.57332 23454
2	- 0.24991 055	18.0590169730	25.6329 61486
3	0.05519 968	8.6347608925	21.0996 30827
4	-0.00976 004	0.2677737343	3.95849 69228
5	0.00107 857		

A decrease of thermal conductivity with depth is observed in all models except in the deepest zone corresponding to the lower crust, where thermal conductivity is practically constant (Figure 3). In the upper zones, the decrease of thermal conductivity is less important when taking into account the pressure effect. This confirms the work of Seipold (1992), who showed that thermal conductivity of a granite sample decreases regularly with depth. At contacts between geological units, thermal conductivity shows drastic discontinuities due to conductivity contrasts.

The influence of the thermal conductivity model on the shapes of the geotherms was also investigated (Figure 3). It appears that, for very low surface heat flow values, the difference between the three models is negligible. With increasing heat flow the geotherms diverge and in the ex–
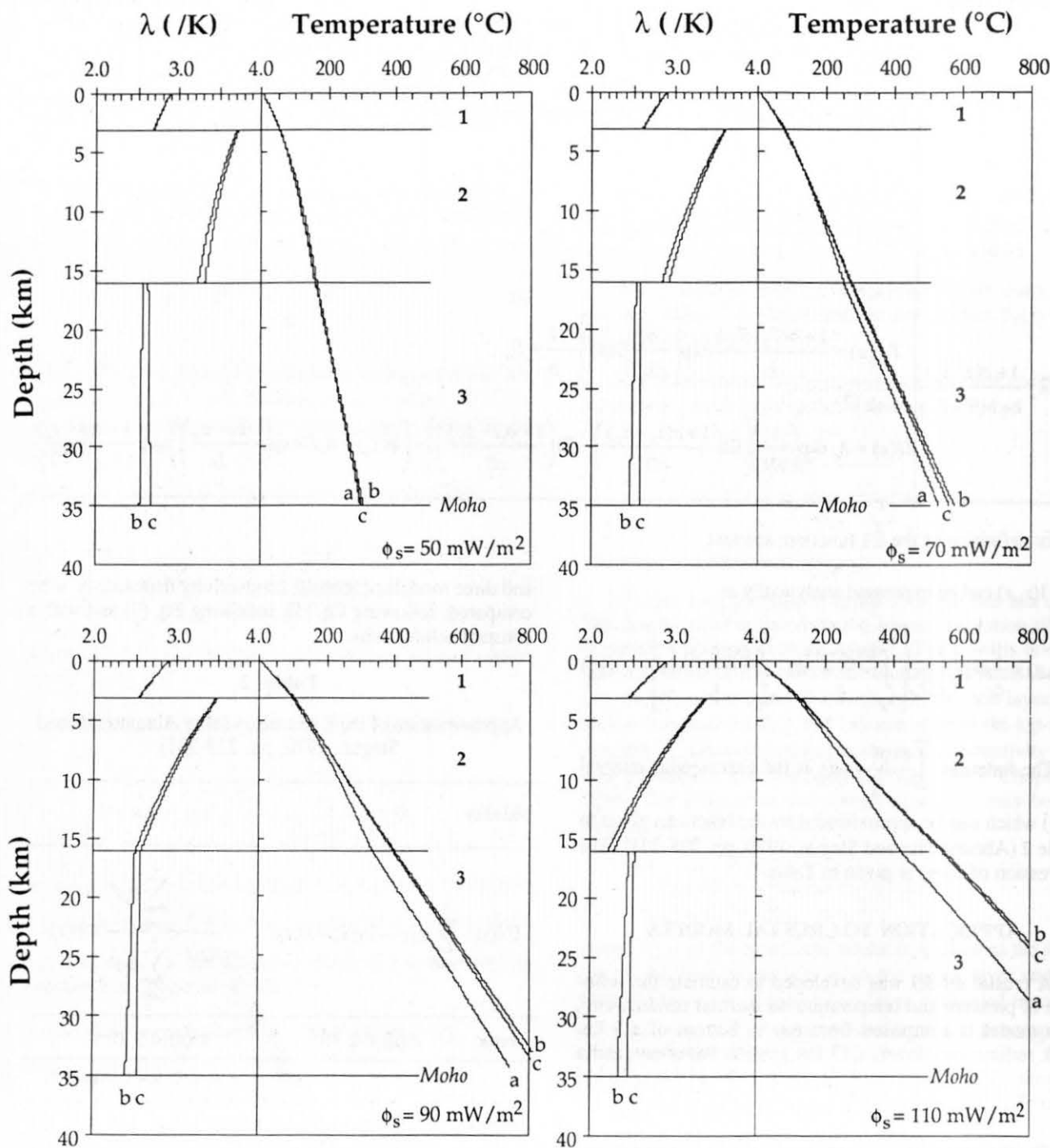

Fig. 3. Variation of thermal conductivity λ (W/mK) and temperature T (°C) with depth z (km) for surface heat flow ϕ_S ranging from 50 to 110 mW/m². Labels a, b and c correspond to models of dependence of the thermal conductivity: constant, temperature dependent and pressure + temperature dependent. Layers number 1, 2 and 3 refer to the sedimentary cover, the granitic layer and the granulitic lower crust.

Table 3

Thermophysical parameters used in the crust model
(Stegena and Meissner, 1985; Chapman, 1986).

		Sedimentary cover	Granitic layer	Lower crust
Lithology		sandstone	granite	granulite
Thickness (km)		3	13	19
Thermal conductivity (W cm^{-1} °C^{-1})		2.9	4.0	6x10^{-3}
T-z dependance	b (°C^{-1})	1.5x10^{-3}		1.0x10^{-4}
	c (km^{-1})	1.5x10^{-4}		
Heat production	A$_o$ (μWm^{-1})	2.8	5.0	0.4
	D (km^{-1})	8		+∞
Surface conditions	Heat flow (mW m^{-2})	50 / 70 / 90/ 110		
	Temperature (°C)	5		

treme case the difference in temperatures at the Moho can reach 100°C. Thermal conductivity discontinuities are responsible for visible changes of the geotherm shape.

In the uppermost layers accessible to drilling, the computed temperature is quite similar for the three models of thermal conductivity, whatever the surface heat flow. In Earth temperature modelling dealing with the shallower levels, thermal conductivity can therefore be taken as independent of temperature and pressure, corresponding to the measured values for surface conditions.

CONCLUSIONS

Thermal conductivity is an essential parameter for characterizing heat transport by conduction only. Conductivity measurements are usually made under surface conditions but the *in situ* values depend on the physical (pressure-temperature) properties of the medium.

The geotherms obtained by including the pressure effect are close to those made by considering only the temperature effect. The errors are small and probably less significant than the errors in the thermal properties for mainly surface heat flow. The pressure effect on thermal conductivity can be neglected in future calculations for sub-surface-layers, but in cases of high surface heat flow this effect can be important below 5 km depth. In all cases, the effect of pressure and temperature on conductivity values is important below the Conrad discontinuity.

ACKNOWLEDGMENTS

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