Thermal regime and rheological properties of the Ossa-Morena Zone
and South Portuguese Zone, Iberian Massif, Southern Portugal

by

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B.Sc. (Hons.)

A thesis submitted to the Faculty of Graduate Studies and Research
in partial fulfillment of the requirements for the
degree of Master of Science

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A handwritten signature in black ink, appearing to read 'G. Rapalli', written over a horizontal line.

Dr. G. Rapalli, Thesis Supervisor

A handwritten signature in black ink, appearing to read 'G. Dix', written over a horizontal line.

Dr. G. Dix, Chair, Department of Earth Sciences, Carleton University

Abstract

Geotherms for the Ossa-Morena Zone (OMZ) and the South Portuguese Zone (SPZ) in the Variscan Iberian Massif are subject to many uncertainties, arising mainly from poor constraints on surface heat flow and crustal heat production. Previous attempts have used either the step model with heat production derived from seismic wave velocities, or the exponential model. Realistic estimates have been obtained for the OMZ ($T_M = 500\text{--}600\text{ }^{\circ}\text{C}$, where T_M is Moho temperature). However, estimates for the SPZ are too high ($T_M = 800\text{--}900\text{ }^{\circ}\text{C}$), require an unrealistically high value of Moho heat flow, and contradict magnetotelluric observations that imply a lower crust without partial melting.

In order to reduce the uncertainties on temperature distributions, families of geotherms are calculated for OMZ and SPZ for surface heat flows of 60 and 80 mW m^{-2} , respectively, for a three-layered crust, allowing heat production in each layer to vary within realistic limits. Only geotherms that satisfy upper-bound constraints on Moho temperature ($T_M < 700\text{ }^{\circ}\text{C}$) and Moho heat flow ($q_M < 30\text{ mW m}^{-2}$) are retained for analysis. This approach leads to the determination of the best-fitting crustal heat production values, provides an estimate of the temperature uncertainties, and requires that Moho heat flow in both zones be consistent with values in other Variscan Massifs.

The geotherms obtained for the OMZ do not differ significantly from previous estimates. Moho temperatures cluster around 550–590 $^{\circ}\text{C}$. Best-fitting heat production values in the three crustal layers are 1.8, 0.8, and 0.3 $\mu\text{W m}^{-3}$, respectively. These values are consistent with measured upper crustal values in the OMZ and average crustal compositions in various tectonic settings. In the SPZ, on the other hand, acceptable Moho temperatures (590–630 $^{\circ}\text{C}$), together with the upper bound on Moho heat flow, require a highly radioactive upper crust of “granitic” composition: best-fitting values are 3.3, 0.7, and 0.3 $\mu\text{W m}^{-3}$, respectively. Therefore, excluding transient effects due to post-Variscan tectonothermal events, the long-wavelength difference in surface heat flow between the OMZ and the SPZ can be attributed to lateral variations in upper crustal heat production.

Average geotherms and inferred compositions of crustal layers (constrained by seismic velocities and heat production) are used to infer the variations of rheological properties with depth in the OMZ and the SPZ. Rheologically weak layers, present at the base of the upper, middle, and lower crust under hydrostatic pore fluid conditions ($\lambda = 0.4$, where λ is the ratio between pore fluid pressure and lithostatic pressure) thin or disappear under fluid-saturated conditions ($\lambda = 0.9$). Rheological lithospheric thickness (100–115 km) and total strength ($S = 10^{12}\text{--}10^{13}\text{ N m}^{-1}$) are within the usual ranges for Palaeozoic massifs.

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1. Introduction

This thesis deals with the determination of the thermal regime and rheological properties of the crust in the Ossa-Morena (OMZ) and South Portuguese (SPZ) zones of the Iberian Massif, Southern Portugal.

1.1 Importance of thermal and rheological state of the crust

The interior heat of the Earth is transmitted to its surface mainly by three mechanisms: radiation, convection, and conduction. In the Earth's lithosphere, conduction of heat generally dominates (Clauser and Huenges, 1995). Conduction involves movement of heat without movement of mass. The heat transferred by conduction is a function of the thermal diffusivity and the temperature gradient. Terrestrial heat flow at the Earth's surface provides highly valuable information about the thermal conditions and processes at depth (e.g. Čermák and Rybach, 1991). In particular, the rheological behaviour of lithospheric plates depends strongly on their internal thermal regime. Thus, integrated studies of heat flow and lithospheric structure are best suited to address some of the basic questions in geodynamics.

1.2 Factors of uncertainty

There is a great deal of uncertainty inherent in the values of surface heat flow as well as in the determination of thermal and rheological properties. Evaluation of heat flow disturbances demonstrates that heat conduction (lateral or vertical) from a strong heat source in the upper crust has a large impact on the measured surface heat flow (Förster and Förster, 2000). Surface heat flow on land is measured using boreholes or exploration wells. The temperature gradient and the thermal conductivity of the country rock are measured and then multiplied to obtain the surface heat flow, according to Fourier's law of conduction, $q_i = -K \partial T / \partial x_i$, where q_i is the surface heat flow, K is the thermal conductivity, and $\partial T / \partial x_i$ is the temperature gradient (index notation and the summation convention are used in this thesis). Since field measurements can be both costly and time consuming, there is generally very poor coverage of measurements, and consequently, a high degree of uncertainty.

Near-surface groundwater circulation can cause perturbations in surface heat flow and increase the uncertainty in heat flow measurements. The simultaneous flow of heat and groundwater is a coupled process. The flow of water is mainly controlled by the pattern of hydraulic gradients, but additional flow can be induced by the presence of a thermal gradient (Freeze and Cherry, 1979). Conductive transport of heat occurs even in static groundwater. Convective transport occurs when heat is carried along by flowing groundwater. In most

systems convective effects exceed conductive effects. The geothermal gradient is greater near the surface in discharge areas than in recharge areas, it increases with depth in recharge areas, and decreases with depth in discharge areas. The effects of groundwater circulation on surface heat flow are more pronounced in regions in which the depth of groundwater flow is of the same order of magnitude as the lateral extent, such as in sedimentary basins (Freeze and Cherry, 1979).

Groundwater circulation adjacent to recently emplaced plutons can also cause sizable perturbations in surface heat flow.

The principal thermal parameters that introduce uncertainty into the calculation of geotherms are thermal conductivity and heat production. Thermal conductivity is a measure of the ability of a particular material to conduct heat (Bates and Jackson 1984). The Earth is a poor conductor; therefore, we expect values of thermal conductivity for most rocks and minerals at room pressure and temperature conditions to be relatively low ($<5 \text{ Wm}^{-1}\text{K}^{-1}$). Typical assigned values of thermal conductivity in the crust are around $2.0\text{-}3.0 \text{ Wm}^{-1}\text{K}^{-1}$ (Clauser and Huenges, 1995; Mareschal et al., 2000). Thermal conductivity decreases with an increase in temperature or porosity and increases slightly with an increase in pressure. To complicate matters, thermal conductivity may vary by as much as a factor of two to three for any given rock type due to the natural variation of a rock's mineral content, physical properties, and diagenesis (Clauser and Huenges 1995).

Heat production values can be estimated based on rock type, but due to large differences in the concentrations of radiogenic elements within a single rock type, this method introduces a high level of uncertainty. Heat production values can also be measured directly from the amounts of radiogenic elements within a specific rock sample. Depending on the scope and detail of a project, it may be more appropriate to assume an average value of heat production for a region rather than attempting to map out small-scale variations.

Although the uncertainties in rheological parameters are large, the main features of rheological profiles (strength envelopes) can be established with an order-of-magnitude degree of confidence (Ranalli, 1995). The variation of strength with depth depends primarily on the temperature gradient of the region, the thickness of the crust, and the average composition of the crustal layers. In the brittle regime, the strength of a layer is based on the tectonic regime (type of faulting), the average density, gravity, depth, and pore fluid pressure. In the ductile regime, the creep properties are estimated using the rheological parameters of rocks together with estimated compositions. Parameter values listed in various compilations (e.g. Kirby and Kronenberg, 1987; Ranalli and Murphy, 1987; Ranalli, 1995) are only indicative, and error limits can be qualitatively assessed to be large. Nonetheless, first-order differences in materials can be determined based on their creep activation energy, which reflects ‘softness’ under crustal conditions. Quartz-rich rocks, whose activation energies are of the order of 100-150 kJ mol⁻¹, are softer than plagioclase-rich rocks, whose activation energies are

200-250 kJ mol⁻¹. Ultrabasic rocks, with activation energies generally in excess of 300 kJ mol⁻¹, are the hardest (Ranalli, 1995).

1.3 Plan of the thesis

This thesis is divided into seven chapters. The first chapter introduces the topic, describes the main factors involved, and outlines the plan of the thesis. The second chapter discusses the general characteristics of Variscan Massifs, gives a brief geological description of the Ossa-Morena and South Portuguese Zones, and describes the available geophysical data for the two zones.

The third and fourth chapters comprise the thermal section of this thesis. In chapter three, the fundamental equations are derived, the thermal parameters are discussed, and previous studies of uncertainties in temperature determinations are examined. In chapter four, one-dimensional heat flow through the crust is examined in detail for both zones, and a simplified two-dimensional geothermal profile across the two zones is produced. Poorly defined thermal parameters are allowed to vary within realistic limits, populations of geotherms under various assumptions are calculated for the OMZ and SPZ, and results are expressed as averages $\pm 2\sigma$ (σ is the standard deviation) of geotherms satisfying a given surface heat flow and upper limits on Moho temperature and heat flow. The Moho heat flow is not given as a boundary condition but is a result of the calculation. Since the main focus is on the effects of uncertainties in thermal parameters on the

temperature distribution, this thesis concentrates primarily on the one-dimensional case, in order to limit the number of possible tradeoffs in the system. This approach is justified since the limited data available do not allow detailed two-dimensional analysis, except for the narrow zone of high heat flow separating the OMZ and SPZ (see Correia and Ramalho, 1999; Correia and Šafanda, 2002). The results are consistent with those obtained using different forward modelling techniques (Correia and Šafanda, 2002), and provide a first-order analysis of the effects of uncertainties in geothermal parameters on the estimated temperature distribution. In addition, an estimate of the thickness of the thermal lithosphere is given.

The fifth and sixth chapters make up the rheological section of the thesis. Chapter five describes the construction of rheological profiles (strength envelopes) and discusses error margins and the effects of pre-existing faults on the rheology of the lithosphere. In chapter six, the rheological properties of the OMZ and SPZ are determined for each of the thermal cases and displayed using standard rheological profiles. A two-dimensional rheological profile is produced based on the two-dimensional geothermal profile constructed in chapter four. In addition, an estimate of the thickness and strength of the rheological lithosphere is given.

A summary of the main conclusions and an accompanying discussion is provided in chapter seven. The relevant tables and figures can be found following each chapter, while references are listed at the end of the thesis.

2. Geology and geophysics of the Southern Portuguese Variscan Massif

2.1 General characteristics of Variscan Massifs

The term Variscan (sometimes Hercynian) refers to the orogenic episode between late Devonian and late Carboniferous time (see e.g. Eguíluz et al., 2000). Across several regions in Europe, the Variscan fold belt is an area of Late Paleozoic deformation and metamorphism (~ 400-250 Ma). Once a wide mountain belt, it is now composed of a number of crystalline massifs of various sizes outcropping in recently uplifted units as shown in Fig. 2.1 (Ager, 1980). In undisturbed and topographically lower regions, the Paleozoic basement is buried under a Mesozoic-Cenozoic platform cover. In the majority of Variscan massifs, the thickness of the crust varies from 30 to 40 km and the characteristic surface heat flow is around 50-60 mW m⁻² (Čermák et al., 1991). Compared with the Precambrian cratons (shield areas) of the world, the heat flow within the massifs is higher and more varied, and a number of local anomalies reflect the heterogeneity of the crust. Localized zones of thinned crust where the Moho is relatively shallow usually exhibit an elevated heat flow value of up to 70 mW m⁻² (Čermák, 1979).

One specific example of a Variscan massif is the Bohemian massif in Central Europe. At the northwestern edge of the Bohemian massif, along the border between Germany and the Czech Republic, is a large NE trending antiformal megastructure called the Erzgebirge. From a data set of temperature logs and

thermal conductivity measurements, surface heat flow in the Erzgebirge was determined to be in the range 61-112 mW m⁻² (Förster and Förster, 2000). The highest surface heat flow values can be correlated with the presence of strongly radiogenic (high heat producing) granite intrusions within a metamorphic basement. From the surface heat flow data, two distinct groups of values can be distinguished: values in the range of 61-71 mW m⁻² were measured from sites not on granite plutons, and higher values of the order of 75-99 mW m⁻² were measured from sites on granite plutons (Förster and Förster, 2000). Measured values of surface heat flow were corrected by as much as 20 mW m⁻² to compensate for the variation of conductive heat transfer due to compositional heterogeneity in the upper crust. The mantle heat flow (i.e. flowing across the Moho) in the Erzgebirge structure was determined to be in the range 20-30 mW m⁻², based on heat budget calculations from crustal models derived from seismic and gravimetric surveys (Förster and Förster, 2000).

2.2 Ossa-Morena Zone and South Portuguese Zone: geological data

The Ossa-Morena zone (OMZ) and the South Portuguese zone (SPZ) are the main geotectonic units found in southern Portugal (Correia and Ramalho, 1999). These two zones are part of the Variscan Iberian Massif (VIM) located on the western half of the Iberian Peninsula, see Fig. 2.2 (Fernández et al., 1998). The Iberian Peninsula consists of a core of the Variscan chain, bordered to the northeast and

southeast by segments of the Alpine foldbelt, and to the west by the Atlantic Ocean (Julivert et al., 1980). The Variscan Iberian Massif is the largest outcrop of the Variscan belt in western Europe. It is mainly made up of metasediments and granitic rocks that are Precambrian and Palaeozoic in age (Fernández et al., 1998). The Massif is crossed by Variscan structures showing longitudinal zonation trending northwest/southeast.

The Ossa-Morena Zone is characterized by Precambrian and lower Paleozoic rocks that show intense deformation and widespread synorogenic magmatism. The OMZ includes an upper Proterozoic basement showing inliers of high-pressure metamorphic rocks and a Paleozoic series including bimodal volcanics of a typical intracontinental rift character (Monteiro Santos et al., 1999). Granitoid rocks outcrop in a transitional domain to the northeast while to the southwest there is an increase of basic intrusions with dominant calc-alkaline chemistry. Most of the major structural features are elongate and trend approximately northwest/southeast (Dallmeyer and Quesada, 1992).

The South Portuguese Zone is composed of late Paleozoic rocks and acid volcanism is more common. The SPZ includes late Devonian – late Carboniferous sediments and volcanics deposited in an intracontinental transtensional setting (Monteiro Santos et al., 1999). Metamorphism is of low grade, mostly within the greenschist facies, and plutonism is not as extensive as in the Ossa-Morena Zone (Correia and Ramalho, 1999). The South Portuguese

terrane was deformed in a transpressional regime during the upper Carboniferous (Monteiro Santos et al., 1999).

A major overthrust separates the OMZ to the northeast from the SPZ to the southwest. Named the Ferreira-Ficalho Overthrust, it is a late Paleozoic, south-vergent, low-angle thrust fault which dips shallowly to the northeast. Hanging-wall rocks of the Ossa-Morena Zone overlie rocks of the Beja-Acebuches Ophiolite and related oceanic sequences (Dallmeyer and Quesada, 1992). Across the two zones, there is a conspicuous tectonic and paleogeographic polarity; the ages of the flysch formations and of the main deformation episode become younger towards the southwest (Correia and Ramalho, 1999; Correia and Šafanda, 2002).

2.3 Geophysical data

From seismic profiles, the crust of the OMZ and SPZ can be divided into three main layers: upper, middle, and lower (Monteiro Santos et al., 1999). Both zones show an increase in seismic velocity with depth. Seismic velocity is a function not only of temperature and pressure, but also of rock type. Increased seismic velocities in the middle and lower crustal layers indicate that each of the crustal layers is composed of a different rock type. The transition from the SPZ to the OMZ is very clear on seismic profiles, particularly in the uppermost crust.

The area is characterized by several geophysical anomalies. The different magnetic signatures of the zones are apparent in the aeromagnetic survey of Portugal (Miranda et al., 1988). The SPZ is characterized by small amplitude, medium to large wavelength (tens of km) negative anomalies contrasting with the OMZ that shows medium amplitude, small wavelength (< 10 km) positive magnetic anomalies, mainly correlated to the Beja gabbroic rocks (Monteiro Santos et al., 1999). The general trend of these anomalies is to the northeast.

Magnetotelluric (MT) studies are scarce in the southern part of Portugal. Correia (1994) and Jones and Correia (1995) have studied the intersection of the Messejana fault and the Ferreira-Ficalho overthrust in the transition between the OMZ and SPZ. From a 3D interpretation of the data, the authors conclude that the region is characterized by the existence of high electrical resistivity blocks embedded in more conductive formations. An MT survey carried out in the SPZ (Almeida et al., 1996; Monteiro Santos et al., 1997) revealed an unknown deep fault. More recently, high-quality magnetotelluric soundings were carried out across the boundary between the Ossa-Morena and South Portuguese zones (Monteiro Santos et al., 1999) in part to confirm the existence of an old suture at the transition between the two zones. The most important result from magnetotellurics for the purposes of this thesis is that electrical conductivities exclude partial melting in the lower crust. The high-conductivity/low-resistivity values that were obtained at lower and middle crustal depths (20-40 km) (Monteiro Santos et al., 1999) could be explained by large amounts of partial

melting, up to 27 vol.% melt to obtain a resistivity of 1 Ωm . However, 27 % partial melting is unrealistically high and therefore this mechanism can be excluded. In addition, collision processes in the region stopped 300 Ma ago (cf. Fonseca and Ribeiro, 1993) and therefore active melting processes at present are unlikely. Taking this along with other factors into account, the authors (Monteiro Santos et al., 1999) conclude that the presence of graphite is a more plausible explanation for low resistivity values at lower crustal depths.

There have been some gravity surveys done in the Ossa-Morena and South Portuguese zones. In the SPZ, Bouguer gravity anomalies are positive with large wavelengths. In contrast, the OMZ shows both positive and negative, small wavelength anomalies (Torres and Lisboa, 1988). However, a more detailed gravity interpretation is lacking.

Fig. 2.1 Map of the Variscan massifs of Western Europe (from Ager, 1980). The location of the OMZ and SPZ is outlined in red.

Fig. 2.2 Map of the Iberian Peninsula (from Fernández et al., 1998).

3. Crustal temperatures: general considerations

3.1 Heat transfer in the lithosphere: fundamental equations

Assuming that thermal conduction is the relevant mechanism of heat transfer, the heat conduction equation is set up by considering an elemental parallelepiped of infinitesimal volume $dV = dx_1 dx_2 dx_3$ and faces normal to the coordinate axes (see Fig. 3.1; cf. e.g. Carslaw and Jaeger, 1959; Ranalli, 1995). The net heat flow through the faces perpendicular to the x_2 -direction is

$$\left(q_2 + \frac{\partial q_2}{\partial x_2} dx_2 \right) dx_1 dx_3 - q_2 dx_1 dx_3 = \frac{\partial q_2}{\partial x_2} dV \quad (3.1)$$

and similarly for each of the two remaining pairs of faces perpendicular to the x_1 - and x_3 -directions. The net flow of heat from the elemental volume is therefore $(\partial q_i / \partial x_i) dV$.

At equilibrium, the heat flow from the elemental volume must be equal to the heat produced within dV , plus any change in the heat content of dV . Advective terms are absent if it is assumed that there is no movement of the volume. Denoting the heat production function (per unit mass and time) by $F(x_1, x_2, x_3, t)$ and any change in the heat content of dV by $\partial Q / \partial t$, we may therefore write

$$\frac{\partial q_i}{\partial x_i} dV = -\frac{\partial Q}{\partial t} + \rho F dV \quad (3.2)$$

where the minus sign signifies that an outflow of heat larger than the heat generated results in a decrease of heat content. Using Fourier's law of heat conduction (assuming isotropy)

$$q_i = -K \partial T / \partial x_i \quad (3.3)$$

where K is the thermal conductivity, which establishes the linear proportionality between heat flow q_i and temperature gradient in a thermally isotropic medium, and the fact that the change in heat content is related to the temperature change by $\partial Q / \partial t = c\rho(\partial T / \partial t) dV$, where c and ρ are the specific heat and density, respectively, equation (3.2) becomes

$$\frac{\partial}{\partial x_i} \left(-K \frac{\partial T}{\partial x_i} \right) dV = -c\rho \frac{\partial T}{\partial t} dV + \rho F dV \quad (3.4)$$

which, dividing by dV and assuming K constant, reduces to

$$K \nabla^2 T = c\rho \frac{\partial T}{\partial t} - \rho F \quad (3.5)$$

This equation is the general form of the heat conduction equation. If the heat generation rate per unit volume $A(x_1, x_2, x_3, t)$ rather than per unit mass F is used, the term ρF in equations (3.4) and (3.5) is replaced by A . Using the definition of thermal diffusivity, $\kappa = K/\rho c$, equation (3.5) can be written as

$$\kappa \nabla^2 T = \frac{\partial T}{\partial t} - \frac{A}{\rho c} \quad (3.6)$$

In a lithospheric plate, heat is transferred by conduction, except in anomalous areas where magmatic or hydrothermal processes play a significant role. The temperature distribution in the lithosphere can therefore be determined by solving the relevant form of the heat transfer equation. For the case of a continental lithosphere, where z denotes the vertical coordinate (positive downwards), and transient effects can be neglected (if the last tectonothermal event is sufficiently old: ≥ 100 Ma), temperature is a function of depth only

$$K \frac{d^2 T}{dz^2} + A(z) = 0 \quad (3.7)$$

The heat generation function $A(z)$ is subject to observational constraints and, in general, decreases with increasing depth. This decrease can be modelled by either a stepwise or an exponential relation. To begin with, an exponential form may be assumed (e.g. Čermák, 1982; Chapman and Furlong, 1992)

$$A = A_0 \exp(-z/d) \quad (3.8)$$

where d is a characteristic depth of the order of 10 ± 5 km, and A_0 is the heat production rate of the uppermost crustal layer. Equation (3.7), with $A(z)$ given by (3.8), can be integrated with boundary conditions $q = -q_0$, $T = T_0$ at the surface and $q = -q_r$ for $z \rightarrow \infty$ (q_r being the heat flow from below the upper layer). The solution is

$$T = T_0 + \frac{A_0 d^2}{K} [1 - \exp(-z/d)] + \frac{q_r}{K} z \quad (3.9)$$

or, in terms of observed heat flow,

$$T = T_0 + \frac{(q_0 - q_r)d}{K} [1 - \exp(-z/d)] + \frac{q_r}{K} z \quad (3.10)$$

where q_r is the reduced heat flow, given by $q_r = q_0 - dA_0$. Equations (3.9) and (3.10) are the required solution to the heat conduction equation in the continental lithosphere if the heat generation is assumed to decrease exponentially with depth. They permit the computation of $T(z)$ in terms of parameters which are either directly measurable or can be inferred from observation.

There are, however, several assumptions built into the preceding argument. For a start, thermal conductivity is not constant, but varies with rock type, temperature,

and pressure. The thermal conductivity of five broad classes of rocks (metamorphic, acid igneous, basic igneous, “average” crust, and ultrabasic (mantle), as defined by Clauser and Huenges, 1995), corrected for temperature and pressure effects, are illustrated in Fig. 3.2. The applied temperature correction is based on the relation

$$K = \frac{K_0}{1 + bT}$$

where K_0 is the thermal conductivity (in $\text{Wm}^{-1}\text{K}^{-1}$) of the material at room pressure and temperature, b is an empirical parameter ($b = 0.0015 \text{ } ^\circ\text{C}^{-1}$ for common rock types at temperatures lower than about $1000\text{-}1200^\circ\text{C}$; Kukkonen 1998), and T is the temperature (in $^\circ\text{C}$). An alternate form of this relation is

$$K = a + \frac{b}{(350 + T)}$$

where a and b are experimentally determined parameters valid for temperatures up to approximately $1200 \text{ } ^\circ\text{C}$ (Clauser and Huenges, 1995) and T is the temperature (in $^\circ\text{C}$). The pressure correction is minor; once pores are closed, an empirical upper limit is a 10% increase in K at the depth where $T = 700 \text{ } ^\circ\text{C}$ (Ranalli, personal communication). If we assume an adiabatic increase in temperature with depth, and therefore pressure, the pressure correction can be

approximated by a 1.2% increase in the temperature-corrected thermal conductivity for every 100 °C increase from room temperature (20 °C).

In addition, radioactive heat generation depends variously on depth, from exponential to stepwise (i.e. constant in each layer). From this point forward, a stepwise decrease in heat production will be assumed to be more accurate than the exponential model (Ranalli, personal communication). A different method for determining the temperature distribution with depth is to consider the lithosphere as consisting of a number of distinct compositional layers, each with a given heat generation and thermal conductivity (e.g. Chapman and Furlong, 1992). Using this approach, the solution of equation (3.7) for the i -th layer ($i = 1, 2, \dots n$) is

$$T_i = T_{0i} + \frac{q_{0i}}{K_i} z - \frac{A_i}{2K_i} z^2 \quad (3.14)$$

where T_{0i} and q_{0i} are temperature and heat flow at the top of the layer, and depth is measured from the top of the layer. Thus, the temperature $T(z)$ can be obtained for any structure consisting of n layers.

3.2 Thermal parameters: surface heat flow, heat production, and thermal conductivity

Surface heat flow is one of the most important thermal parameters because it can be determined from measurements of temperature gradient and thermal conductivity. It is the main variable from which a geotherm for a given tectonic region is estimated. Surface heat flow is measured using boreholes and exploration wells. Worldwide heat flow measurements show that the mean surface heat flow in continental areas is 57 mW m^{-2} , whereas in oceans it is 66 mW m^{-2} (e.g. Sclater et al., 1980; Fernández et al., 1998). In the continental lithosphere, a general pattern of decreasing heat flow with increasing tectonothermal age has been recognized. Usually, surface heat flow varies from about $40\text{-}50 \text{ mW m}^{-2}$ in stable Precambrian shields to more than 120 mW m^{-2} in recently active tectonic regions (Ranalli, 1991). For regions that have experienced a recent tectonothermal event (within the last 100 Ma), the assumption of steady-state conditions is inaccurate and introduces additional errors (see e.g. Ranalli, 1995). The main factors affecting the surface heat flow are: heat production in the upper crustal layers enriched in radioactive elements and its variation with depth, heat flow from below the upper crustal layers, variation of thermal conductivity with depth, and the tectonic history of the region. Additional factors contributing to the variability of surface heat flow are related to near-surface processes such as the flow of groundwater, erosion, and sedimentation (Ranalli, 1995). The uncertainties involved in determining the

measured surface heat flow are considerable. For some heat flow measurements, the standard deviation is greater than 100% of the average value (Fernández et al., 1998), but usually it is within 10-20% of the average value.

Heat production in the upper crustal layers is one of the main factors affecting surface heat flow. Heat producing isotopes belong to incompatible elements and are therefore concentrated in the upper crust. It is generally recognized that heat production, on the whole, decreases with increasing depth; however, the precise form of this relation is unknown and locally variable. Although an exponential decrease is roughly compatible with observation, other forms are possible, including a stepwise decrease in a layered model (e.g. Ranalli, 1991). The leading source of uncertainty in estimates of heat production is the variable distribution of heat sources within crustal materials. Chemical and mineralogical variations within a single rock type make heat production estimates difficult.

Thermal conductivity and the geothermal gradient are the two quantities that control surface heat flow according to Fourier's law of heat conduction. Thermal conductivity is both pressure and temperature dependent, as previously discussed, and can significantly affect the curvature of the geotherm within a tectonic region. The thermal conductivity of crustal materials is usually about $2\text{--}3 \text{ W m}^{-1} \text{ K}^{-1}$ (Ranalli, 1991). Thermal conductivity can be measured experimentally in the laboratory. The most commonly used technique to determine thermal conductivity in a solid rock specimen is the steady-state comparison method

(Beck, 1988). In this method, heat is passed through both a reference material, for which the thermal conductivity is known, and the unknown specimen. Assuming that transverse heat losses are negligible, which is usually the case, the amount of heat flowing along the system can be determined by finding the temperature gradient in the reference material and then using this value of heat flow to determine the conductivity of the unknown specimen, having first found its temperature gradient. If the apparatus is properly designed, thermal equilibrium can be established within 5-10 minutes. As a result, this method gives experimental values of thermal conductivity quickly and accurately, with inaccuracies of $< 5\%$ (Beck, 1988).

3.3 Previous studies of uncertainties in temperature determinations

The uncertainty of temperature estimates in the crust becomes progressively greater with depth (Chapman and Furlong, 1992). In the uppermost crust, temperature can be directly measured or extrapolated from the temperature gradient. Unfortunately, beyond depths of a few kilometers, the temperature is less certain and depends on the model of heat transfer and on the accuracy of estimates of thermal conductivity and heat production. Careful consideration of the variations of thermal conductivity and heat generation with depth can slightly reduce the margins of error. The effects of parameter uncertainties are seldom studied in geothermal models. Nonetheless, it has been noted that calculated

temperatures may be very sensitive to the choice of input data (Jokinen and Kukkonen, 1999a).

Previous studies using random or stochastic modelling have been presented by Nielsen (1987) and Wang (1990) for investigations of the linear heat flow-heat production relationship (i.e., the correlation between heat production of the uppermost crust and heat flow), and by Lamontagne and Ranalli (1996) for geotherm estimation in a seismic area. Jokinen and Kukkonen (1999a) investigated the possibility of using random simulations of the lithospheric thermal regime in analyzing the accuracy of the calculated temperature and heat flow in terms of *a-priori* information on the thermal parameters.

Random modelling (sometimes called also Monte Carlo sampling of *a-priori* models) differs from stochastic simulation in the sense that no spatial autocorrelation is assumed to exist in the studied parameters. Use of Monte Carlo techniques for the thermal parameters in inversion of temperature and heat flow data is discussed by Jokinen and Kukkonen (1999b). The Monte Carlo method has been found to be useful in thermal inversion studies, and it removes at least partly the subjective judgment and parameter choices always present in forward modelling (Jokinen and Kukkonen, 2000). However, any model is only as good as the input data and basic assumptions behind it, and a lot of uncertainty is still related to the thermal properties of crustal materials.

In general, continental lithospheric geotherms carry considerable uncertainties of the order of $\pm 100\text{-}200\text{ }^{\circ}\text{C}$ at the Moho (cf. Ranalli, 1995). Much of this is related to uncertainties in heat flow. Regional variations in Moho heat flow can be as large as $30 - 40\text{ mW m}^{-2}$ (Čermák 1982). Temperatures and temperature gradients in the lower crust are very sensitive to heat flow because they must adjust to allow the sub-crustal heat flow as well as heat generated within the crust to be conducted to the surface (Chapman and Furlong, 1992). Compositional heterogeneities within the crust can also contribute to uncertainties in temperature by producing strong lateral temperature variations. Temperatures in a compositionally heterogeneous crust may vary by as much as $100\text{ }^{\circ}\text{C}$ at mid-crustal levels along a horizontal distance of 50-75 km (Chapman and Furlong, 1992).

Fig. 3.1 Elemental parallelepiped of volume $dV = dx_1 dx_2 dx_3$ and faces perpendicular to the coordinate axes (from Ranalli, 1995). Heat flow is denoted by q_i .

Fig. 3.2 Thermal conductivity corrected for pressure and temperature effects, see text for explanation.
Rock classes as defined by Clauser & Huenges (1995).

4. Crustal temperatures: OMZ and SPZ

4.1 Determination of thermal parameters: heat flow and heat generation in Southern Portugal

The first heat flow map of the whole Iberian Peninsula and its margins was produced by Fernàndez et al. (1998) (see Fig. 4.1). Correia and Ramalho (1999) present a more detailed heat flow density map of the Ossa-Morena and South Portuguese zones (see Fig. 4.2). In both maps, the average surface heat flow is approximately 60 mW m^{-2} in the OMZ and 80 mW m^{-2} in the SPZ. Although these maps are suitable for a first-order approximation of surface heat flow, data are scarce throughout much of the study area. Thus, any calculations that make use of these approximate values of surface heat flow are limited by the degree of coverage involved in their determination.

In the study by Fernàndez et al. (1998), there are only six discrete heat production values determined for upper crustal rocks in the Ossa-Morena Zone, ranging from $0.2 \text{ } \mu\text{W m}^{-3}$ for gabbros to $2.9 \text{ } \mu\text{W m}^{-3}$ for granites. In the same study, there are no heat production values determined for the South Portuguese zone. The Iberian Peninsula as a whole has an average surface heat production of $2.5 \pm 0.5 \text{ } \mu\text{W m}^{-3}$. This value is approximately the same as the average heat generation rate most often quoted for rocks of granitic composition ($A_G = 2.8 \text{ } \mu\text{W m}^{-3}$; Ranalli, 1995).

4.2 Moho heat flow in Variscan Massifs

The heat flow measured in a stable continental crust can be described by two components: the heat flow from the mantle, and the heat generated by radioactive heat sources within the crust. Local variations in surface heat flow can mostly be explained by variations in the heat production of crustal rocks, in addition to variations produced by hydrogeology and local geological effects. The mantle or Moho heat flow represents the energy outflow from a greater depth, which is the sum of the background heat flow and heat from deep transient thermal perturbations associated with tectogenesis. The Moho heat flow may thus be more dependent on tectonic and magmatic activity than on the age of the overlying crust (Čermák et al., 1991). To evaluate the Moho heat flow, the crustal contribution is subtracted from the observed surface heat flow. Moho and sub-lithospheric heat flow (across the lower boundary of the lithosphere) are about the same because of the low heat production of peridotites ($A_P = 0.02 \mu\text{W m}^{-3}$; Ranalli, 1995).

A preliminary sketch map of the Moho heat flow distribution in Europe was produced by Čermák (1982) based on the compilation of the estimates of q_M published by different authors. Crustal heat production was evaluated by converting average seismic velocity into heat production data in a $2^\circ \times 2^\circ$ grid network, using Rybach and Buntebarth's equation that describes the empirical relationship of heat production and seismic velocity (Rybach and Buntebarth,

1982). The map confirms that the Moho heat flow across Europe varies in the range 15-50 mW m⁻². In the Variscan structures of Central Europe, which include the Bohemian Massif and its northern slopes, the Moho heat flow ranges from 20 to 35 mW m⁻², with an average value of 26 mW m⁻² (Čermák et al., 1991). Moho heat flow is lower under Precambrian shields, ~15-20 mW m⁻² (Čermák, 1982; Drury, 1991; Jaupart et al., 1998), and higher under Cenozoic orogens, ~37-39 mW m⁻² (Čermák et al., 1991) so q_M , at least, if not q_0 , is roughly related to tectonic age.

4.3 Previous studies in OMZ and SPZ

In the last two decades, there has been an attempt to understand the geological and geophysical evolution of southern Portugal and, in particular, there has been an effort to gather geothermal data that will allow the construction of thermal models for the region. Southern Portugal is geologically complex but constitutes one of the best exposures of the Variscan orogeny (Correia and Ramalho, 1999). Heat flow values in the region were estimated by Duque and Mendes-Victor (1993) and by Fernández et al. (1998). The heat flow map presented by the former authors shows a large anomaly located around the SPZ-OMZ suture. The map of the latter authors is a filtered map and does not show any major heat flow anomalies (see also Monteiro Santos et al., 1999).

One dimensional geotherms for the Ossa-Morena and South Portuguese zones were calculated by Correia and Ramalho (1999) using the equation obtained in Chapter 3

$$T = T_0 + \frac{q_0}{K}z - \frac{A}{2K}z^2 \quad (4.1)$$

where T is the temperature at depth z from the top of the layer, T_0 is the temperature at the top of the layer, q_0 is the heat flow from the top of the layer, A is the heat production for the layer, and K is the thermal conductivity. This equation allows the calculation of temperature at depth for a stepwise model in which the lithosphere is approximated as a number of layers, presumably of different rock types, each with a specific value of heat production and thermal conductivity.

From seismic refraction surveys (Mendes-Victor et al., 1993), it has been determined that both the OMZ and the SPZ have a three-layer crustal structure. In the Ossa-Morena zone, the top layer is 12 km thick, the middle layer is 11 km thick, and the bottom layer is 7 km thick, for a total crustal thickness of 30 km. In the South Portuguese zone, the total thickness of the crust is 29 km, with the thickness of the layers being 14, 7, and 8 km respectively. In their study, Correia and Ramalho (1999) obtained heat production values from U-Th-K concentrations in surface samples for the upper crust. In the middle and lower crust, the heat

generation was derived from the empirical relationship of heat production and seismic velocity

$$\ln A = 16.5 - 2.74 v_p$$

where A is heat production (in $\mu\text{W m}^{-3}$) and v_p is the velocity of compressional waves (in km s^{-1}) corrected to 50 MPa (cf. Rybach and Buntebarth, 1982; 1984). Geotherms for the two zones were then calculated using the parameters given in Table 4.1. The resulting geotherms are shown in Fig. 4.3.

Correia and Ramalho's estimates result in a realistic geotherm for the OMZ, with temperatures $< 700^\circ\text{C}$ at the base of the crust, but in an unrealistic geotherm for the SPZ, with Moho temperatures of up to 900°C . Temperatures of this magnitude would indicate partial melting in the lower crust, a condition that has been excluded by magnetotelluric data (Monteiro Santos et al., 1999). Obtaining geotherms with more realistic basal crustal temperatures for the SPZ is one of the main goals of the thermal section of this thesis.

4.4 Justification of parameter ranges and upper limits on T_M , q_M (*)

In the following sections, crustal geotherms are calculated for both the Ossa-Morena and South Portuguese Zones using discrete sampling of parameter space (henceforth denoted by DSPS). This approach provides a number of possible combinations of thermal parameters which are used in calculating the variation of temperature with depth.

To begin with, by adopting the same three-layered crustal structure proposed by Correia and Ramalho (1999), but recognizing that the parameters must be altered to decrease the calculated Moho temperature of the SPZ, a pair of base geotherms is calculated (Case 1 in Table 4.2) using equation (4.1). Heat production rates are chosen based on a combination of measured values in the upper crust and accepted values for average crustal material (Ranalli, personal communication), and constrained by the assumption that the Moho heat flow for both zones must be the same and is likely to be about 30 mW m^{-2} as an upper limit. Heat production rates are related to Moho heat flow as

$$q_M = q_S - \sum_i A_i h_i \quad (4.2)$$

(*) The material in sections 4.4-4.5 has been used in the paper: Ellsworth, C. and Ranalli, G. (2002). Crustal temperatures in the Variscan massif of southern Portugal: an assessment of effects of parameter variations. *Journal of Geodynamics*, **34**, 1-10.

where q_M and q_S are heat flow from the mantle and surface respectively, A is heat production and h is the thickness of layers $i = 1, 2$, and 3 . The average surface heat flow is taken to be 60 mW m^{-2} in the Ossa-Morena Zone and 80 mW m^{-2} in the South Portuguese Zone (Correia and Ramalho, 1999; Fernàndez et al., 1998). The calculation of this pair of geotherms results in one possible unique solution for the thermal regime in the Ossa-Morena and South Portuguese Zones. This pair of geotherms is shown in Fig. 4.4, the parameters are displayed in Table 4.2 (Case 1), and the numerical results are displayed in Table 4.3 (Case 1). The OMZ reaches a temperature of 517°C at a depth of 30 km ; the SPZ reaches a temperature of 548°C at a depth of 29 km . This solution produces fairly realistic temperatures at the base of the crust and requires that the Moho heat flow be 30 mW m^{-2} in both zones.

For the uncertainty analysis, the Moho heat flow boundary condition is dropped, and the variability of calculated geotherms is evaluated as a function of uncertainties in thermal parameters. Three sets of solutions are calculated using equation (4.1), with increasingly narrow constraints. The first set contains geotherms with $T_M \leq 700^\circ\text{C}$ and no upper bound on q_M , the second set contains geotherms with $T_M \leq 700^\circ\text{C}$ and $q_M \leq 40 \text{ mW m}^{-2}$, and the third set contains geotherms with $T_M \leq 700^\circ\text{C}$ and $q_M \leq 30 \text{ mW m}^{-2}$. In all cases, geotherms are calculated with no *a priori* constraints on Moho temperature and heat flow; however, only solutions satisfying the double constraint, $T_M \leq 700^\circ\text{C}$, $q_M \leq 30 \text{ mW m}^{-2}$, from the most exclusive set are retained for analysis.

There is evidence from magnetotelluric observations (Monteiro Santos et al., 1999) that partial melt is not present in the lower crust in southern Portugal. Therefore, the temperature at the Moho should be no more than 700 °C. This is the justification for setting an upper limit of $T_M \leq 700$ °C on the temperature at the base of the lower crust. An upper limit of $q_M \leq 30$ mW m⁻² is set for the heat flow from the mantle because this is a realistic upper limit on Moho heat flow for a Variscan Massif. For other Variscan Massifs, the average Moho heat flow has been estimated at 26 mW m⁻² (Čermák et al., 1991).

The ranges of heat production and thermal conductivity used in this thesis, discussed in the following sections, are within usual accepted values (see e.g. Zoth and Haenel, 1988; Clauser and Huenges, 1995; Fernández et al., 1998).

4.5 One-dimensional, constant K solutions

In the first case in which the DSPS approach is used (Case 2a), in order to analyze the effects of variations in heat production values, the crustal thermal conductivity is taken to be constant, $K = 2.5$ W m⁻¹K⁻¹, which is approximately the weighted average of the layer conductivities used for the base geotherms (this value is considered representative for the continental crust; see Clauser and Huenges, 1995; Mareschal et al., 2000). The heat production rates for the different crustal layers in the Ossa-Morena Zone are allowed to vary in steps of

0.1 as follows (in $\mu\text{W m}^{-3}$): $1.0 < A_1 < 2.0$, $0.4 < A_2 < 1.0$, and $0.1 < A_3 < 0.4$ (see Table 4.2, Case 2a). In the South Portuguese Zone, the heat production rates are varied stepwise within the same ranges as in the OMZ, except that the upper limit in the upper crust (A_1) is increased to $3.5 \mu\text{W m}^{-3}$. This results in 308 and 728 geotherms for the OMZ and SPZ, respectively. When geotherms that do not satisfy Moho heat flow and temperature constraints are dropped, sample sizes are reduced to 92 geotherms for the OMZ and 129 geotherms for the SPZ. Average geotherms for these two zones (calculated on the most restrictive assumptions on T_M , q_M), together with their $\pm 2\sigma$ limits (containing $\sim 95\%$ of accepted geotherms) are shown in Fig. 4.5. Resulting average Moho temperatures are 477 ± 31 °C in the OMZ and 509 ± 36 °C in the SPZ. The best-fitting heat production rates (best-fitting in the sense that the parameters fit the average geotherm) are also shown in Table 4.3 (Case 2a), as are the values of Moho heat flow corresponding to average $\pm 2\sigma$ geotherms. The values of Moho heat flow are obtained from equation (4.2).

In the second case (Case 2b), both heat production and thermal conductivity are allowed to vary for each layer, heat production as in Case 2a and conductivity in both the OMZ and SPZ in steps of 0.1 as follows (in $\text{W m}^{-1} \text{K}^{-1}$): $2.0 < K_1 < 2.5$, $1.8 < K_2 < 2.0$, and $1.6 < K_3 < 1.8$ (see Table 4.2, Case 2b). The lower ranges in the middle and lower crust are chosen to take into account the decrease in thermal conductivity with increasing temperature as previously discussed (cf. e.g. Clauser and Huenges, 1995). The resulting geotherm sample size is 16,632 for the OMZ

and 39,312 for the SPZ. These are reduced to 5130 and 7093 geotherms, respectively, when Moho heat flow and maximum temperature constraints are applied. Resulting average $\pm 2\sigma$ geotherms are shown in Fig. 4.6. Average Moho temperatures are 590 ± 61 °C in the OMZ, and 616 ± 73 °C in the SPZ. Best-fitting (in the sense defined above) heat production rates and thermal conductivities are shown in Table 4.3 (Case 2b), together with the corresponding values of Moho heat flow.

In the third case (Case 2c), weighted averages of the best-fitting thermal conductivities obtained in the previous case (Case 2b) are used as constant crustal conductivities for each zone ($K = 2.1 \text{ W m}^{-1} \text{ K}^{-1}$ for the OMZ; $K = 2.0 \text{ W m}^{-1} \text{ K}^{-1}$ for the SPZ), with heat production varying in the same manner as in the previous two cases (see Table 4.2, Case 2c). 308 and 728 geotherms are initially calculated for the Ossa-Morena and South Portuguese zones respectively. After Moho constraints are applied, the sample sizes are reduced to 82 for the OMZ and 123 for the SPZ. Average and $\pm 2\sigma$ geotherms are shown in Fig. 4.7. Average Moho temperatures are 563 ± 35 °C in the OMZ, and 631 ± 44 °C in the SPZ. Best fitting heat production rates and corresponding values of Moho heat flow are shown in Table 4.3 (Case 2c).

4.6 One-dimensional, $K(T)$ solutions

Since temperature, and to a lesser extent pressure, is known to have an effect on thermal properties, the case is considered where thermal conductivity is temperature dependent according to the relation

$$K = \frac{K_0}{1 + bT} \quad (4.3)$$

where K_0 is the thermal conductivity (in $\text{W m}^{-1} \text{K}^{-1}$) of the material at room temperature (20°C), b is an empirical parameter ($b = 0.0015^\circ\text{C}^{-1}$ for common rock types at temperatures lower than about $1000\text{--}1200^\circ\text{C}$; Kukkonen, 1998), and T is temperature in $^\circ\text{C}$. Using this relation, an analytical solution for the heat conduction equation (3.5) for steady-state conditions ($\partial T/\partial t = 0$) can be obtained (Rybach, 1981)

$$T(z) = \frac{1}{b}(1 + bT_0) \left\{ \exp \left[\frac{b}{K_0} \left(q_0 z - A_0 \frac{z^2}{2} \right) \right] - 1 \right\} \quad (4.4)$$

where b and K_0 are the same as in equation (4.3), q_0 is the heat flow at the top of the layer (in mW m^{-2}), z is the depth from the top of the layer, and A_0 is the heat production at the top of the layer (in this case, assumed constant for each layer and equal to A_i).

In Case 3a, the best-fitting values of thermal conductivity calculated in Case 2b (Table 4.3) are set as K in equation (4.3) and used to calculate K_0 . The average geotherms from Case 2b are used to select an average T for each layer (arithmetic mean of the temperatures within the layer). This calculation results in values (in $\text{W m}^{-1} \text{K}^{-1}$) of $K_{01} = 2.8$, $K_{02} = 3.0$, and $K_{03} = 3.0$ for the Ossa-Morena Zone and $K_{01} = 3.0$, $K_{02} = 3.1$, and $K_{03} = 3.1$ for the South Portuguese Zone. Heat production values are allowed to vary in the same manner as in previous cases (see Table 4.2, Case 3a). From these parameters, 308 and 728 geotherms are initially calculated for the OMZ and SPZ respectively. The same Moho constraints described above are applied and only geotherms with $T_M \leq 700$ °C and $q_M \leq 30$ mW m⁻² are retained for analysis. The resulting average $\pm 2\sigma$ geotherms are shown in Fig. 4.8. For the OMZ, with a sample size of $n = 95$ geotherms, the temperature is 582 ± 51 °C at a depth of 30 km. For the SPZ, with a sample size of $n = 133$ geotherms, the temperature is 594 ± 58 °C at a depth of 29 km. The best-fitting heat production rates and corresponding values of Moho heat flow for average $\pm 2\sigma$ geotherms are given in Table 4.3 (Case 3a).

In Case 3b, K_0 is chosen on the basis of the inferred rock type for each layer. The representative rock type for each layer is determined through a comparison of geophysical parameters such as seismic velocities and heat production values obtained in previous studies of the area (Monteiro Santos et al., 1999; Correia and Ramalho, 1999; Holbrook et al., 1992). In addition, some consideration is given to the surface geology and tectonic setting of the region. For the purpose of this

thesis, the composition of the crustal layers of both the Ossa-Morena and South Portuguese Zones can be approximated by a felsic (“granitic”) upper crust, an intermediate (“quartz dioritic”) middle crust, and a mafic (“mafic granulitic”) lower crust. It is fair to consider the upper crust “granitic” in both zones despite higher heat production in the South Portuguese zone because compositional variations within granites can produce a wide range of heat production rates. The crustal composition of each zone along with seismic velocities (from Correia and Ramalho, 1999) and thermal conductivities at room temperature (values from the compilation by Zoth and Haenel, 1988) are shown in Table 4.4. For both zones, $K_{01} = 3.1$ (upper crust), $K_{02} = 3.0$ (middle crust), and $K_{03} = 2.5 \text{ Wm}^{-1}\text{K}^{-1}$ (lower crust). Heat production is varied in the same way as in previous cases (see Table 4.2, Case 3b). From these parameters, 308 and 728 geotherms are initially calculated for the OMZ and SPZ respectively. After the most restrictive Moho constraints are applied, average geotherms $\pm 2\sigma$ are calculated and the results for each zone are shown in Fig. 4.9. For the OMZ, with a sample size of $n = 95$ geotherms, the average temperature is $557 \pm 51 \text{ }^{\circ}\text{C}$ at a depth of 30 km. For the SPZ, with a sample size of $n = 133$ geotherms, the average temperature is $604 \pm 63 \text{ }^{\circ}\text{C}$ at a depth of 29 km. The best-fitting heat production rates for the average geotherms $\pm 2\sigma$ are given in Table 4.3 (Case 3b) as well as the corresponding values for Moho heat flow.

Fig. 4.10 shows the average geotherms for the OMZ and the SPZ for each of the one-dimensional DSPS cases where thermal conductivity varies stepwise (Case

2a,b,c). This figure allows easier comparison of the differences in the geotherms for the two zones. The geotherms for the OMZ and SPZ diverge in the upper crust reaching a maximum temperature difference at a depth of about $z \cong 12$ km. Below this point, the geotherms in the two zones are roughly parallel and then begin to converge slightly towards the base of the crust. The temperature gradient is higher in the upper crust for the SPZ and roughly parallel between the two zones in the middle and lower crust. From the previous series of figures (Figs. 4.5-4.9), it can be seen that the errors associated with the average geotherms increase with depth through the crust reaching a maximum at the Moho. The average temperature difference between the OMZ and SPZ at the Moho is generally within the 2σ error margins of the geotherms and is therefore not significant. Because T_M is approximately the same for the OMZ and the SPZ, the lithospheric thickness should also be approximately the same. This will be further discussed in an upcoming section.

4.7 Two-dimensional solutions

A two-dimensional profile of the first-order temperature distribution across the two zones is produced using the software “Processing SHEMAT - version 1.1.10” developed by M. Kühn and W.-H. Chiang (2000). The forward calculation of temperature and heat flow was done with the FORTRAN code SHEMAT, version 7.0 authors J. Bartels, C. Clauser, and M. Kühn. SHEMAT (Simulator of HEat

and MAss Transport) is a finite-difference code for simulating steady-state and transient processes in hydro-geothermal reservoirs in two and three dimensions (Clauser, 1988; Clauser and Villinger, 1990). In this thesis, only steady-state, purely conductive simulations were used.

Initially, one-dimensional geothermal profiles are produced for each zone to ensure that results from SHEMAT match those calculated in the analytical solutions presented above. The calculated values of thermal conductivity (K_{0i}) as well as best-fitting values of heat production (A_i) and Moho heat flow (q_M) from Case 3a are inputted into a grid representing a slice of the OMZ 10 km in length, 30 km in depth, and 1 km in width. This results in a temperature of $T_M = 597$ °C at a depth of 30 km. Next, the best-fitting values from Case 3b are inputted into the same size of grid, resulting in a value of $T_M = 561$ °C at 30 km. The same procedure is followed to produce one-dimensional profiles of the SPZ, where the grid represents a section 10 km in length, 29 km in depth, and 1 km in width. The temperature obtained for this zone is $T_M = 625$ °C at a depth of 29 km using the parameters from Case 3a. Using the best-fitting values from Case 3b, a value of $T_M = 606$ °C is calculated at a depth of 29 km. There is a small discrepancy between the temperatures calculated in the analytical solutions (Case 3a, 3b) and those calculated using SHEMAT, reaching maximums of 15 and 4 °C respectively at the base of the Ossa-Morena zone, and 31 and 2 °C respectively at the base of the South Portuguese zone. These temperature differences translate to

errors of less than 5 %. Therefore, the results from SHEMAT can be constructively compared to the analytical results.

Two-dimensional profiles are produced using the best-fitting parameters arrived at in the analytical solutions (see Table 4.3, Case 3a). A grid is produced to represent a slice of the lithosphere running roughly north-south across the OMZ and the SPZ with an assumed horizontal distance of 100 km, a depth of 30 km, and a width of 1 km. The geological structure is defined so that a low-angle thrust fault ($< 30^\circ$) dipping north separates the two zones; the Ossa-Morena Zone to the north overlies the South Portuguese Zone to the south. The basal heat flow must be the same for both zones and should be somewhere between the values of q_M calculated for each zone in Case 3a. Through trial and error, this value is adjusted so that the surface heat flow is as close as possible to 60 mW m^{-2} for the Ossa-Morena Zone and 80 mW m^{-2} for the South Portuguese Zone (after Correia and Ramalho, 1999). The best-fitting solution using the parameters obtained in Case 3a, with a Moho heat flow of $q_M = 27 \text{ mW m}^{-2}$, results in surface heat flow values of $q_S = 60 \text{ mW m}^{-2}$ for the Ossa-Morena Zone and $q_S = 80 \text{ mW m}^{-2}$ for the South Portuguese Zone. The temperature profile produced by this method is shown in Fig. 4.11 (Case 4a). The maximum temperatures reached are 589°C in the Ossa-Morena zone (left side) and 641°C in the South Portuguese zone (right side). The procedure is repeated for the set of best-fitting thermal parameters obtained from Case 3b (see Table 4.3, Case 3b). The best-fitting solution for this case, with a Moho heat flow of $q_M = 27 \text{ mW m}^{-2}$, results in surface heat flow values of

$q_S = 60 \text{ mW m}^{-2}$ for the OMZ, and $q_S = 79 \text{ mW m}^{-2}$ for the SPZ. This second two-dimensional temperature profile (Case 4b) is shown in Fig. 4.12. The maximum basal temperatures reached in this case are $554 \text{ }^\circ\text{C}$ in the Ossa-Morena Zone and $617 \text{ }^\circ\text{C}$ in the South Portuguese Zone. The 2D profile shows clearly that the SPZ crust is hotter than the OMZ crust by generally $\sim 50 \text{ }^\circ\text{C}$, the difference increasing with depth.

4.8 Estimate of thickness of the thermal lithosphere

The thermal lithosphere is defined as the layer where heat transfer is mainly conductive, and temperature is below the wet solidus (Kukkonen and Peltonen, 1999). In this thesis, the lower boundary of the thermal lithosphere is considered to be between the critical temperatures $1200 \text{ }^\circ\text{C}$ (lower bound) and $1350 \text{ }^\circ\text{C}$ (upper bound) (Fowler, 1990; Ranalli, 1995). These temperatures approximate the range of melting temperatures for wet peridotite at upper mantle pressures ($T_m \approx 1500\text{-}1600 \text{ K}$) (Ranalli, 1995). For all the one-dimensional cases considered in this chapter, the calculated average geotherm for each zone is extended to the bottom of the thermal lithosphere. Equation (4.1) is applied to an upper mantle layer of peridotite composition with constant thermal conductivity $K = 3.5 \text{ W m}^{-1} \text{ K}^{-1}$, heat production $A = 0.02 \text{ } \mu\text{W m}^{-3}$ (Ranalli, 1995), and $q_0 = q_M$, $T_0 = T_M$. The basal heat flow is taken to be $q = 26$ and 25 mW m^{-2} for the OMZ and SPZ, respectively (heat flow at the bottom of the lithosphere is less than at the Moho

because of the contribution of subcrustal lithospheric mantle, in this case taken to be about 1.5 mW m^{-2}). The resulting estimated thickness of the thermal lithosphere is summarized in Table 4.5 and displayed in Figs. 4.13 – 4.15 for each of the one-dimensional cases. The thickness of the thermal lithosphere is in the range 121 – 143 km in the Ossa-Morena Zone, and 118 – 141 km in the South Portuguese Zone. The difference in lithospheric thickness between the two zones is not significant. This is to be expected because the temperature difference between the OMZ and the SPZ at the base of the Moho is within the 2σ error margins associated with the respective average geotherms. Since the temperature at the base of the crust in each of the two zones is approximately the same and the upper mantle is considered homogeneous, then it is expected that the OMZ and the SPZ would have the same lithospheric thickness.

Table 4.1. Parameters for Correia and Ramalho's (1999) geotherms.

	Layer	Thickness (km)	Thermal Conductivity K ($\text{W m}^{-1} \text{K}^{-1}$)	Heat Production A ($\mu\text{W m}^{-3}$)
OMZ	1	12	2.7	1.39
	2	11	2.5	0.34
	3	7	2.1	0.12
SPZ	1	14	2.7	0.53
	2	7	2.5	0.43
	3	8	2.1	0.08

Table 4.2. Thermal parameters for the Ossa-Morena Zone (OMZ) and South Portuguese Zone (SPZ).

	A ₁			A ₂			A ₃			K ₁	K ₂	K ₃	N
OMZ													
Case 1	1.4			0.9			0.4			2.7	2.5	2.1	1
Case 2a	1.0, 1.1, 1.2, ..., 2.0			0.4, 0.5, 0.6, ..., 1.0			0.1, 0.2, 0.3, 0.4			2.5	2.5	2.5	308
Case 2b	1.0, 1.1, 1.2, ..., 2.0			0.4, 0.5, 0.6, ..., 1.0			0.1, 0.2, 0.3, 0.4			2.0, 2.1, 2.2, ..., 2.5	1.8, 1.9, 2.0	1.6, 1.7, 1.8	16,632
Case 2c	1.0, 1.1, 1.2, ..., 2.0			0.4, 0.5, 0.6, ..., 1.0			0.1, 0.2, 0.3, 0.4			2.1	2.1	2.1	308
Case 3a	1.0, 1.1, 1.2, ..., 2.0			0.4, 0.5, 0.6, ..., 1.0			0.1, 0.2, 0.3, 0.4			2.8*	3.0*	3.0*	308
Case 3b	1.0, 1.1, 1.2, ..., 2.0			0.4, 0.5, 0.6, ..., 1.0			0.1, 0.2, 0.3, 0.4			3.1*	3.0*	2.5*	308
SPZ													
Case 1	2.9			0.9			0.4			2.7	2.5	2.1	1
Case 2a	1.0, 1.1, 1.2, ..., 3.5			0.4, 0.5, 0.6, ..., 1.0			0.1, 0.2, 0.3, 0.4			2.5	2.5	2.5	728
Case 2b	1.0, 1.1, 1.2, ..., 3.5			0.4, 0.5, 0.6, ..., 1.0			0.1, 0.2, 0.3, 0.4			2.0, 2.1, 2.2, ..., 2.5	1.8, 1.9, 2.0	1.6, 1.7, 1.8	39,312
Case 2c	1.0, 1.1, 1.2, ..., 3.5			0.4, 0.5, 0.6, ..., 1.0			0.1, 0.2, 0.3, 0.4			2.0	2.0	2.0	728
Case 3a	1.0, 1.1, 1.2, ..., 3.5			0.4, 0.5, 0.6, ..., 1.0			0.1, 0.2, 0.3, 0.4			3.0*	3.1*	3.1*	728
Case 3b	1.0, 1.1, 1.2, ..., 3.5			0.4, 0.5, 0.6, ..., 1.0			0.1, 0.2, 0.3, 0.4			3.1*	3.0*	2.5*	728

Units... A ($\mu\text{W m}^{-3}$), K ($\text{W m}^{-1} \text{K}^{-1}$), N is the number of geotherms; the sample size satisfying q_M , T_M constraints is shown in the figures and Table 4.3. * ... For case 3a, 3b, K_{01} values are shown.

Table 4.3. Best-fitting thermal parameters and results for the Ossa-Morena Zone (OMZ) and South Portuguese Zone (SPZ).

	A ₁	A ₂	A ₃	K ₁	K ₂	K ₃	T _M	q _M	n
OMZ									
Case 1	1.4	0.9	0.4	2.7	2.5	2.1	517	30.0	1
Case 2a	1.9	0.7	0.4	2.5	2.5	2.5	477 ± 31	26.8 ± 3.6	92
Case 2b	1.8	0.8	0.3	2.2	1.9	1.7	590 ± 61	27.3 ± 3.9	5130
Case 2c	1.8	0.8	0.3	2.1	2.1	2.1	563 ± 35	27.0 ± 3.4	82
Case 3a	1.8	0.8	0.3	2.8*	3.0*	3.0*	582 ± 51	27.4 ± 3.5	95
Case 3b	1.8	0.8	0.3	3.1*	3.0*	2.5*	557 ± 51	27.4 ± 3.7	95
SPZ									
Case 1	2.9	0.9	0.4	2.7	2.5	2.1	548	30.0	1
Case 2a	3.3	0.7	0.3	2.5	2.5	2.5	509 ± 36	26.4 ± 4.1	129
Case 2b	3.3	0.7	0.3	2.2	1.9	1.7	616 ± 73	26.5 ± 3.8	7093
Case 2c	3.2	0.8	0.3	2.0	2.0	2.0	631 ± 44	26.3 ± 3.9	123
Case 3a	3.3	0.7	0.3	3.0*	3.1*	3.1*	594 ± 58	26.6 ± 4.0	133
Case 3b	3.3	0.7	0.3	3.1*	3.0*	2.5*	604 ± 63	26.6 ± 4.2	133

Units... A ($\mu\text{W m}^{-3}$), K ($\text{W m}^{-1} \text{K}^{-1}$), T ($^{\circ}\text{C}$), q (mW m^{-2}), n is the number of geotherms that satisfying q_M, T_M constraints.

* ... For case 3a, 3b, K_{0i} values are shown.

Table 4.4. Crustal composition of the OMZ and SPZ for Case 3b.

	Layer	V_P (km s ⁻¹)	Rock Type	K_i (Wm ⁻¹ K ⁻¹)
<u>OMZ</u>	1	6.1	Felsic	3.1
	2	6.3	Intermediate	3.0
	3	6.8	Mafic	2.5
<u>SPZ</u>	1	6.1	Felsic	3.1
	2	6.2	Intermediate	3.0
	3	7.0	Mafic	2.5

Table 4.5. Estimates of the thickness of the thermal lithosphere.

	Thickness of OMZ (in km)		Thickness of SPZ (in km)	
	$Z_{\min}$	$Z_{\max}$	$Z_{\min}$	$Z_{\max}$
Case 1	126	148	124	147
Case 2a	132	154	129	152
Case 2b	115	137	113	136
Case 2c	118	141	112	135
Case 3a	116	138	117	140
Case 3b	120	142	115	138
Average	121	143	118	141

Fig. 4.1 Map of surface heat flow in the Iberian Peninsula (from Fernández et al., 1998).

Fig. 4.2 Map of surface heat flow for the Ossa-Morena and South Portuguese Zones (from Correia & Ramalho, 1999).

Fig. 4.3 Geotherms from Correia and Ramalho (1999).

Fig. 4.4 Case 1 - geotherms for the Ossa-Morena and South Portuguese Zones.

Fig. 4.5 Average $\pm 2\sigma$ geotherms for Case 2a.

A) OMZ

B) SPZ

Fig. 4.6 Average $\pm 2\sigma$ geotherms for Case 2b.

Fig. 4.7 Average $\pm 2\sigma$ geotherms for Case 2c.

A) OMZ

B) SPZ

Fig. 4.8 Average $\pm 2\sigma$ geotherms for Case 3a.

Fig. 4.9 Average $\pm 2\sigma$ geotherms for Case 3b.

Fig. 4.10 Average geotherms for the OMZ and SPZ in each of the 1D DSPS cases where K varies stepwise.

Fig. 4.11 Two-dimensional temperature profile for Case 4a along a 100 km long, 1 km wide N-S transect across the boundary between the OMZ and SPZ. Black line indicates the approximate location of the fault that separates the two zones. Temperature contours are in 50° increments.

Fig. 4.12 Two-dimensional temperature profile for Case 4b along a 100 km long, 1 km wide N-S transect across the boundary between the OMZ and SPZ. Black line indicates the approximate location of the fault that separates the two zones. Temperature contours are in 50° increments.

Fig. 4.13 Thickness of the thermal lithosphere: minimum thickness at 1200 °C and maximum thickness at 1350 °C.

A) Case 1

B) Case 2a

Fig. 4.14 Thickness of the thermal lithosphere: minimum thickness at 1200 °C and maximum thickness at 1350 °C.

A) Case 2b

B) Case 2c

Fig. 4.15 Thickness of the thermal lithosphere: minimum thickness at 1200 °C and maximum thickness at 1350 °C.

A) Case 3a

B) Case 3b

5. Rheological profiles (strength envelopes): general considerations

Rheology is the branch of physics dealing with the deformation and flow of materials (Ranalli, 1995). In practical terms, rheology is the study of a material's deformational response to applied stress. A number of rheological behaviours exist and the type of response depends not only on the intrinsic characteristics of the material under consideration, but also on external parameters, such as pressure, temperature, and time.

5.1 Construction of rheological profiles

Lithospheric thickness is controlled by temperature, whereas crustal thickness is controlled by composition (Ranalli, 1995). The interaction of composition and temperature result in rheological stratification of the lithosphere. The variations of lithospheric strength with depth can be displayed as rheological profiles (also termed strength envelopes). Rheological profiles are constructed by combining lithologic and structural information (from geological and geophysical data) with estimated geotherms (see e.g. Ranalli, 1991). The construction of rheological profiles requires an approximate knowledge of the composition and rheology of lithospheric layers and an estimate of temperature as a function of depth. The rheology of the lithosphere is estimated on the basis of pore-pressure dependent frictional failure in the brittle regime, and power-law steady-state creep in the

ductile regime (Ranalli and Murphy, 1987). In the brittle regime, a linear frictional failure criterion applies to practically all rocks and can be written in terms of stress difference, overburden pressure, and pore fluid pressure as

$$\sigma_1 - \sigma_3 = \alpha \rho g z (1 - \lambda) \quad (5.1)$$

where σ_1 and σ_3 are maximum and minimum compressive stresses (their difference is termed the critical stress difference), ρ is the average density of the overlying material, g is acceleration of gravity (9.8 m s^{-2}), z is depth, λ is the pore fluid factor (the ratio of pore fluid pressure to overburden pressure), and α is a numerical parameter that is dependent on the regionally dominant type of faulting. The value of α for ideally oriented cohesionless pre-existing faults with friction coefficient $\mu = 0.75$ is 3.0 for thrust faults, 0.75 for normal faults, and 1.2 for strike-slip faults (Ranalli, 1995). The frictional failure criterion is a pressure-dependent, temperature-independent limiting condition, which for the most part does not depend on rock type (Ranalli, 1991). Conversely, the creep strength of rocks in the ductile regime is a function of both rock type and temperature. Creep strength can be defined as the flow stress necessary to maintain a given steady-state strain rate (Ranalli, 1991). In the ductile regime, in materials deforming by power-law creep, the creep strength is given by

$$\sigma_1 - \sigma_3 = \left(\dot{\varepsilon} / A_D \right)^{1/n} \exp(E/nRT) \quad (5.2)$$

where $(\sigma_1 - \sigma_3)$ is the critical stress difference, $\dot{\epsilon}$ is the strain rate, R is the gas constant ($8.3 \text{ J mol}^{-1} \text{ K}^{-1}$), T is absolute temperature, and A_D , n , and E are the Dorn parameter, stress exponent, and creep activation energy, respectively - material parameters which are approximately stress- and temperature-independent (Ranalli and Murphy, 1987).

A rheological profile plots critical stress difference versus depth at a given constant strain rate. If the critical stress difference for frictional sliding calculated by equation (5.1) is less than the creep strength calculated by equation (5.2), failure by frictional sliding will predominate; in the opposite case, ductile flow will occur (Ranalli and Murphy, 1987). Rheological layers can be identified within the lithosphere where the failure of lithospheric materials changes from brittle frictional sliding to ductile creep and vice versa. The vertical variations of rheological properties are therefore determined on the basis of the deformation laws of lithospheric materials.

5.2 Error margins and effects of pre-existing faults

Temperature uncertainties do not play a role in the calculation of critical stress for brittle failure, but they can have a sizable effect on the calculation of ductile failure. The hotter a material is, the more susceptible it is to deformation by ductile creep (Ranalli, 1995). As well, the depth of transitions between brittle and

ductile deformation can be affected by temperature uncertainties. In addition to the contribution of uncertainty from temperature estimates, the accuracy of the calculated creep strength depends on the experimental uncertainty (typically 10-20%) related to the determination of creep parameters (Ranalli, 1991). Creep strength in silicate rocks is roughly inversely proportional to silica content. Quantitative confidence limits cannot be precisely assigned; however, the differences among the principal classes of rocks are well established and sufficiently robust to withstand experimental uncertainties.

The presence of pre-existing faults can significantly affect the frictional strength. In general, although somewhat dependent on orientation, frictional coefficient, and cohesion, pre-existing faults tend to require a lower critical stress difference for reactivation than that required for new faults to form (see Ellsworth, 2000). Along a pre-existing plane of weakness – most commonly a fault, but also a plane of schistosity, layering, etc. – the cohesive strength (~ 10 MPa) can be up to an order of magnitude less than the cohesion that must be overcome for a new fracture to form (50-100 MPa). This is relevant in the brittle, upper part of the crust, where the temperature is less than half of the melting temperature, as this upper layer tends to be highly fractured. For example, at a depth of 10 km, a pre-existing plane of weakness ideally oriented at 26.6° from the direction of maximum stress with $\mu_0 = 0.75$, $\lambda = 0.4$, and $S_0 = 10$ MPa, requires a critical stress difference of 129 MPa to be reactivated as a normal fault. At the same depth, a new normal fault with $\mu = 0.75$, $\lambda = 0.4$, and $S = 100$ MPa, requires a

critical stress difference of 219 MPa to form at an orientation of 26.6° from the direction of maximum stress (Ellsworth, 2000). The equation used in this thesis (eqn. 5.1) takes this into account by assuming that brittle layers are thoroughly prefactured, and contain cohesionless pre-existing planes of weakness of all orientations. This is standard convention for the majority of rheological studies and is a realistic assumption for Paleozoic terrain such as that found in the study area.

6. Rheology of the crust in OMZ and SPZ

6.1 Selection of rheological parameters

Based on the correlation of best-fitting seismic velocities and heat production values with compilations for various rock types (eg. Holbrook et al., 1992), the crustal structure of the Ossa-Morena and South Portuguese zones can be approximated by a felsic (granitic) upper crustal layer, an intermediate (quartz diorite) middle crustal layer, and a mafic (mafic granulite) lower crustal layer. A fourth layer, representing the upper mantle with an average composition of peridotite, represents the mantle part of the lithosphere. Rheological parameters can then be determined based on rock type (Ranalli, 1995). The chosen rheological parameters for the Ossa-Morena and South Portuguese zones are listed in Table 6.1. The upper crust of the SPZ has a higher average value of heat production than the OMZ. This variance can be attributed to a higher concentration of radioactive elements within the granites of the SPZ. As mentioned in a previous section, there can be a wide variation in both the mineral composition and the concentration of elements within a single rock type, so it is not unusual for “granitic rocks” of different compositions to have different values of heat production.

6.2 One-dimensional rheological profiles of OMZ and SPZ

Rheological profiles are produced for each of the one-dimensional cases discussed in the thermal section. First, equation (5.1) is applied to determine the stress difference ($\sigma_1 - \sigma_3$) (in MPa) necessary for brittle failure, given parameters $\alpha = 0.75$ (normal faulting), $\rho = 2.8 \text{ kg m}^{-3}$ (the average density of continental crust), and $g = 9.8 \text{ m s}^{-2}$. Even though seismic data for the region provides poor constraints on source mechanisms, assuming the study area to be in an extensional tectonic setting gives a minimum estimate of strength (Ranalli, 1995). Brittle failure is calculated for both hydrostatic pore fluid conditions ($\lambda = 0.4$) and nearly lithostatic pore fluid conditions ($\lambda = 0.9$). Hydrostatic conditions imply that the pore fluid pressure at a given depth is equal to that of a column of water extending from the surface to that depth; near-lithostatic conditions imply fluid overpressures approaching the rock overburden pressure. Secondly, equation (5.2) is used to calculate the stress difference necessary for ductile creep to occur using a constant strain rate $\dot{\epsilon} = 10^{-15} \text{ s}^{-1}$ (a typical “low” tectonic strain rate), T (in degrees Kelvin) from the average geotherm calculated in each of the thermal cases, and rheological parameters A_D , n , and E as given in Table 6.1 for each rock type. On a plot of stress difference (on a logarithmic scale) versus depth, the lower of the two critical stress differences is plotted for each depth, resulting in a “Christmas Tree” pattern of stronger and weaker rheological layers.

The rheological profiles calculated for the Ossa-Morena Zone at hydrostatic conditions ($\lambda = 0.4$) are shown in Fig. 6.1. Case 1 (A) shows the presence of thin (< 3 km) rheologically weak ductile layers at the base of the upper, middle, and lower crust. The transition from brittle to ductile failure in the upper mantle occurs at a depth of ~ 40 km for a composition of wet peridotite, and at ~ 50 km for a composition of dry peridotite. In Case 2a (B), thin rheologically weak ductile layers are present at the base of the upper and middle crustal sections. The transition from brittle to ductile failure in the upper mantle occurs at depths of 45 and 60 km for wet and dry mantle compositions, respectively. In Case 2b (C), weak ductile layers ~ 5 km thick are evident at the base of the upper, middle, and lower crust. For a composition of "wet" peridotite, the entire upper mantle will fail by ductile creep, while for "dry" peridotite, the transition from brittle to ductile failure occurs at ~ 45 km of depth. In Case 2c (D), rheologically weak ductile layers up to 6 km thick are apparent at the bottom of the upper, middle, and lower crust. The transition from brittle to ductile failure in the upper mantle occurs at depths of ~ 35 and 50 km for wet and dry compositions, respectively. In Case 3a (E), weak ductile layers of between 2 and 5 km are evident at the base of the upper, middle, and lower crust. The transition from brittle to ductile failure in the upper mantle occurs at 30 km of depth for a composition of "wet" peridotite, and at ~ 45 km for "dry" peridotite. In Case 3b (F), there are thin (< 3 km) rheologically weak layers at the base of the upper, middle, and lower crust. The change in deformation response from brittle failure to failure by ductile creep

occurs at depths of ~35 and 50 km in the upper mantle for wet and dry compositions, respectively.

The rheological profiles for the Ossa-Morena Zone under nearly lithostatic conditions ($\lambda = 0.9$) are shown in Fig. 6.2. For Case 1 (A), there are no weak ductile layers present in the crust. The transition from brittle to ductile failure in the upper mantle occurs at depths of ~50 and 65 km for compositions of "wet" and "dry" peridotite, respectively. In Case 2a (B), there is a very thin (~1 km) ductile layer at the base of the upper crust for a composition of "wet" granite. The transition from brittle to ductile failure in the upper mantle occurs at ~55 km for "wet" peridotite, and at ~70 km for "dry" peridotite compositions. In Case 2b, (C), weak ductile layers (< 3 km thick) are present at the base of the upper and middle crust. The upper mantle transition from brittle to ductile failure occurs at ~40 and 55 km for wet and dry mantle compositions, respectively. In Case 2c (D), thin rheologically weak ductile layers are present at the base of the upper and middle crust. The transition from brittle to ductile failure in the upper mantle occurs at 45 km for "wet" mantle and 60 km for "dry" mantle. In Case 3a (E), thin ductile layers (2-3 km thick) are present at the base of the upper crust for a composition of "wet" granite and at the base of the middle crust for a composition of quartz diorite. The transition from brittle to ductile failure in the upper mantle occurs at depths of 45 and 60 km for wet and dry compositions, respectively. In Case 3b (F), there are no rheologically weak layers in the crust and the change in

deformation response from brittle to ductile failure occurs in the upper mantle at depths of 50 and 65 km for "wet" and "dry" peridotite compositions, respectively.

The rheological profiles for the South Portuguese Zone at hydrostatic conditions ($\lambda = 0.4$) are shown in Fig. 6.3. In Case 1 (A), there are weak layers 2-7 km thick at the base of the upper, middle, and lower crust. The transition from brittle to ductile failure occurs at 35 and 50 km in the upper mantle for wet and dry mantle compositions, respectively. In Case 2a (B), there are weak layers at the base of the upper and middle crust approximately half the thickness of the crustal units. In the upper mantle, the transition from brittle to ductile failure occurs at a depth of ~40 km for "wet" peridotite and at ~55 km for "dry" peridotite. In Case 2b (C), thick (~6 km) rheologically weak ductile layers are present in the upper, middle, and lower crust. For "wet" compositions, ductile creep will predominate over brittle failure in the entire upper mantle and for "dry" compositions, the transition depth is ~40 km. In Case 2c (D), the deformation response changes from brittle failure to failure by ductile creep at around 6-7 km of depth in the upper crust. Ductile creep then predominates down to the depth of the Moho. In the upper mantle, brittle failure occurs for a composition of "dry" peridotite down to a depth of ~40 km. For Case 3a (E), thick (5-7 km) rheologically weak ductile layers are present at the base of the upper, middle, and lower crust. For "wet" compositions, ductile creep will predominate over brittle failure in the entire upper mantle and for "dry" compositions, the transition from brittle to ductile failure occurs at a depth of ~45 km. In Case 3b (F), rheologically weak ductile layers ~5 km thick

are present at the base of the upper, middle, and lower crust. The entire upper mantle will fail by ductile creep for "wet" peridotite compositions and the transition from brittle to ductile failure for "dry" peridotite occurs at a depth of ~40 km.

The rheological profiles for the South Portuguese Zone at nearly lithostatic conditions ($\lambda = 0.9$) are shown in Fig. 6.4. In Case 1 (A), a weak ductile layer, for a composition of "wet" granite, is present at the base of the upper crust. The transition from brittle to ductile failure in the upper mantle occurs at ~50 and 65 km for wet and dry compositions, respectively. In Case 2a (B), the upper crust contains a weak ductile layer at its base for "wet" granite. In the upper mantle, the transition from brittle to ductile failure occurs at ~50 and 65 km for "wet" and "dry" peridotite, respectively. For Case 2b (C), thin rheologically weak ductile layers are present at the base of the upper, middle, and lower crust. The transition from brittle to ductile failure in the upper mantle occurs at a depth of 40 km for "wet" mantle and at a depth of ~55 km for "dry" mantle. In Case 2c (D), rheologically weak ductile layers (2-7 km thick) are present at the base of the upper, middle, and lower crust. The transition from brittle to ductile failure in the upper mantle occurs at depths of ~40 and 55 km for wet and dry compositions, respectively. In Case 3a (E), rheologically weak layers (<5 km thick) are present at the base of the upper and middle crust. In the upper mantle, the transition from brittle to ductile failure occurs at 40 and 55 km for wet and dry mantle compositions, respectively. In Case 3b (F), a weak ductile layer ~4 km thick is

evident at the base of the upper crust for a composition of "wet" granite. The transition from brittle to ductile failure in the upper mantle occurs at ~40 km of depth for "wet" compositions and ~55 km of depth for "dry" compositions.

Some basic observations can be made about these four groups of rheological profiles. The depth of the brittle to ductile transition in the upper mantle is comparable for a given zone and pore fluid factor as is the overall shape and appearance of the profile. The South Portuguese Zone has more and thicker rheologically weak ductile layers present at the base of the crustal units than does the Ossa-Morena Zone. For both zones, there are fewer and thinner weak layers present for nearly lithostatic conditions than for hydrostatic conditions.

It should be kept in mind that rheological profiles are only first-order approximations. Uncertainties cannot be assessed quantitatively; however, thin layers ($\leq 2\text{-}3$ km) of a given rheology are likely to lie within error margins.

6.3 Two-dimensional rheological profiles

The two-dimensional temperature data produced in the thermal cases 4a and 4b are used to construct two-dimensional rheological profiles for the Ossa-Morena and South Portuguese Zones. The same geometry previously defined for the thermal model is assumed; a 100 km long, 1 km wide transect that runs

approximately north-south across the boundary between the OMZ and SPZ.

Other than for its effects on temperature distribution, the Ferreira-Ficalho Overthrust (FFO) that separates the two zones is ignored. If the coefficient of friction along this pre-existing plane of weakness is less than 0.75, the rheological strength along the overthrust would be lower than that predicted for the surrounding rock.

By combining the rheological strength calculated for vertical slices taken every 10 km along the horizontal distance of the transect, a grid is produced showing numerically the critical stress difference ($\sigma_1 - \sigma_3$) (in MPa) required for failure at each horizontal distance and corresponding depths. The two-dimensional rheological profile for Case 4a, using a pore fluid factor of $\lambda = 0.4$ and “dry” compositions for the upper crust and upper mantle, is shown in Fig. 6.5. In the blue zones, brittle failure (failure by frictional sliding) requires a lower critical stress difference than ductile failure (failure by ductile creep) and will occur preferentially. In the red zones, the opposite is true and ductile failure will predominate. In Fig. 6.5, weak ductile layers 2-6 km thick are apparent at the base of the upper, middle, and lower crust. Fig. 6.6 shows the 2-D rheological profile for Case 4a, with the pore fluid factor increased to $\lambda = 0.9$ and using “wet” compositions for the upper crust and upper mantle. Brittle failure is much more prevalent in this figure than in the previous profile. Rheologically weak ductile layers at the base of the crustal units are generally no more than 2 km in thickness

and are not continuous in the middle or lower crust. The transition from brittle to ductile failure in the upper mantle occurs at depths of 35-45 km.

The 2-D rheological profile for Case 4b under “dry” conditions ($\lambda = 0.4$, “dry” compositions of upper crust and mantle) is shown in Fig. 6.7. In this profile, there are rheologically weak layers present at the base of the upper, middle, and lower crustal units. All three crustal ductile layers are continuous across the profile with a shared maximum thickness of 5 km at the right (South) side of the profile. The weak layer at the base of the upper crust increases substantially in thickness (from 1 km to 5 km) at 60 km of horizontal distance. The transition from brittle to ductile failure in the upper mantle occurs between 40 and 50 km of depth. Fig. 6.8 shows the two-dimensional rheological profile for Case 4b under “wet” conditions ($\lambda = 0.9$, “wet” compositions of upper crust and mantle). Brittle failure dominates most of this profile with ductile layers present at the base of the upper and middle crust only at the far right of the profile. The transition from brittle to ductile failure in the upper mantle occurs between 35 and 50 km of depth, with a dip to the North.

6.4 Thickness and strength of the rheological lithosphere

Rheological profiles allow the identification of a *rheological lithosphere*, defined as the material above the 1 MPa strength isoline in the upper mantle, below which

there are no further jumps in strength (Ranalli, 1991). The rheological lithosphere can be defined as the layer that behaves as a ‘rigid’ plate on top of a ductile layer that flows (Kukkonen and Peltonen, 1999).

In order to make an estimate of the thickness of the rheological lithosphere in the Ossa-Morena and South Portuguese zones, the depth is determined at which the rheological strength is approximately equal to 1 MPa. Since the bottom layer of the lithosphere is upper mantle material, the rheological properties of peridotite (from Ranalli, 1995) listed in Table 6.1 are used to calculate creep strength (equation 5.2) down to depths of around 100 km. For each of the one-dimensional thermal cases (Case 1-3b), the average geotherm is extended into an upper mantle layer of peridotite composition using equation (4.1) with basal heat flow $q = 26$ and 25 mW m^{-2} for the OMZ and SPZ, respectively, constant thermal conductivity $K = 3.5 \text{ W m}^{-1} \text{ K}^{-1}$, and heat production $A = 0.02 \text{ } \mu\text{W m}^{-3}$. From the extended geotherms, the rheological strength is calculated and a maximum and minimum thickness is estimated for dry and wet peridotite, respectively.

Using this method, the average thickness of the rheological lithosphere is estimated at 103 – 116 km for the Ossa-Morena Zone and 100 – 113 km for the South Portuguese Zone. Specific estimates of the lithospheric thickness for each of the one-dimensional thermal cases are given in Table 6.2. As is the case for the thermal lithosphere, the difference in thickness of the rheological lithosphere between the two zones is not significant. This relates back to the fact that Moho

temperatures for the OMZ and the SPZ are nearly the same and the upper mantle is considered homogeneous beneath the two zones. Taking the 10MPa isoline as the lower limit of the rheological lithosphere would decrease estimates of lithospheric thickness by about 20 km.

The rheological stratification of the lithosphere affects its overall mechanical properties. Total lithospheric strength, S , can be defined as

$$S = \int_0^H \sigma(z) dz \quad (6.1)$$

where H is the thickness of the rheological lithosphere (as defined above) and $\sigma(z)$ is the strength ($\sigma_1 - \sigma_3$) as a function of depth – the function displayed in standard rheological profiles. Lithospheric strength decreases with increasing geotherm for a given crustal thickness and composition. However, both thickness and composition affect lithospheric strength, since the ductile strength of rocks usually increases with decreasing SiO_2 content. Pore fluid pressure also affects lithospheric strength because it is used in the calculation of the brittle strength of rocks. An increase in pore fluid pressure causes a decrease in lithospheric strength. The total strength of oceanic lithosphere varies from 10^{12} to more than 10^{13} N m^{-1} with increasing age. Continental lithosphere has roughly similar limits, with minimum strength in rift systems and maximum strength in Precambrian shields (Ranalli, 1991).

Estimates of the total lithospheric strength in the Ossa-Morena and South Portuguese Zones are obtained through numerical integration of the rheological profiles produced in Section 6.2. Results of this integration, using only the curves representing “dry” compositions in the upper crust and upper mantle, are shown in Table 6.3. The average strength of the Ossa-Morena Zone under hydrostatic conditions ($\lambda = 0.4$) is of the order of $2 \times 10^{13} \text{ N m}^{-1}$. At nearly lithostatic conditions ($\lambda = 0.9$), the average strength is $5 \times 10^{12} \text{ N m}^{-1}$. The average strength of the South Portuguese Zone is slightly lower, of the order of $1 \times 10^{13} \text{ N m}^{-1}$ under hydrostatic conditions, and $4 \times 10^{12} \text{ N m}^{-1}$ at nearly lithostatic conditions. The above estimates represent maximum lithospheric strengths since only “dry” ductile parameters are considered. High pore fluid pressures have a greater affect on the brittle layers; however, use of “wet” ductile parameters would decrease lithospheric strength by as much as $1.5 \times 10^{12} \text{ N m}^{-1}$.

Table 6.1. Rheological parameters for the Ossa-Morena Zone (OMZ) and South Portuguese Zone (SPZ) (Ranalli, 1995).

	Upper crust		Middle crust	Lower crust		Upper mantle	
<u>OMZ</u>	Granite		Quartz diorite	Mafic granulite	Peridotite	dry	wet
	dry	wet					
	1.8×10^{-9}	2.0×10^{-4}	1.3×10^{-3}	1.4×10^{-4}	2.5×10^4	2.0×10^3	
	A_D ($\text{MPa}^{-n} \text{s}^{-1}$) n E (kJ mol^{-1})	3.2 1.9 123	2.4 219	4.2 445	3.5 532	4.0 471	
<u>SPZ</u>	Granite		Quartz diorite	Mafic granulite	Peridotite	dry	wet
	dry	wet					
	1.8×10^{-9}	2.0×10^{-4}	1.3×10^{-3}	1.4×10^4	2.5×10^4	2.0×10^3	
	A_D ($\text{MPa}^{-n} \text{s}^{-1}$) n E (kJ mol^{-1})	3.2 1.9 123	2.4 219	4.2 445	3.5 532	4.0 471	

Table 6.2. Estimates of the thickness of the rheological lithosphere.

	Thickness of OMZ (in km)		Thickness of SPZ (in km)	
	$Z_{\min}$	$Z_{\max}$	$Z_{\min}$	$Z_{\max}$
Case 1	107	120	105	118
Case 2a	113	126	111	124
Case 2b	97	110	95	108
Case 2c	101	113	93	106
Case 3a	98	111	98	111
Case 3b	102	114	97	110
Average	103	116	100	113

Table 6.3. Estimates of the total lithospheric strength.

	Strength of OMZ (in N m^{-1})		Strength of SPZ (in N m^{-1})	
	$\lambda = 0.4$	$\lambda = 0.9$	$\lambda = 0.4$	$\lambda = 0.9$
Case 1	2.0×10^{13}	4.8×10^{12}	1.6×10^{13}	4.3×10^{12}
Case 2a	2.5×10^{13}	6.3×10^{12}	2.1×10^{13}	5.8×10^{12}
Case 2b	1.3×10^{13}	4.0×10^{12}	1.1×10^{13}	3.5×10^{12}
Case 2c	1.6×10^{13}	4.8×10^{12}	0.9×10^{13}	3.3×10^{12}
Case 3a	1.5×10^{13}	4.3×10^{12}	1.3×10^{13}	4.0×10^{12}
Case 3b	1.7×10^{13}	4.5×10^{12}	1.3×10^{13}	4.0×10^{12}
Average	2×10^{13}	5×10^{12}	1×10^{13}	4×10^{12}

Fig. 6.1 Rheological profiles for the Ossa-Morena Zone under hydrostatic conditions ($\lambda = 0.4$). Dashed lines represent "wet" compositions, solid lines represent "dry" compositions.

Fig. 6.2 Rheological profiles for the Ossa-Morena Zone under nearly lithostatic conditions ($\lambda = 0.9$).

Fig. 6.3 Rheological profiles for the South Portuguese Zone under hydrostatic conditions ($\lambda = 0.4$).

Fig. 6.4 Rheological profiles for the South Portuguese Zone under nearly lithostatic conditions ($\lambda = 0.9$).

Fig. 6.5 2D rheological profile for Case 4a at hydrostatic conditions ($\lambda = 0.4$). "Dry" compositions are assumed for the upper crust and upper mantle. Blue zones indicate where failure by frictional sliding predominates, red zones indicate where failure by ductile creep predominates.

Fig. 6.6 2D rheological profile for Case 4a at nearly lithostatic conditions ($\lambda = 0.9$). "Wet" compositions are assumed for the upper crust and upper mantle. Blue zones indicate where failure by frictional sliding predominates, red zones indicate where failure by ductile creep predominates.

Fig. 6.7 2D rheological profile for Case 4b at hydrostatic conditions ($\lambda = 0.4$). "Dry" compositions are assumed for the upper crust and upper mantle. Blue zones indicate where failure by frictional sliding predominates, red zones indicate where failure by ductile creep predominates.

Fig. 6.8 2D rheological profile for Case 4b at nearly lithostatic conditions ($\lambda = 0.9$). "Wet" compositions are assumed for the upper crust and upper mantle. Blue zones indicate where failure by frictional sliding predominates, red zones indicate where failure by ductile creep predominates.

7. Discussion and conclusions

7.1 Thermal state of the crust in Southern Portugal

The geotherms obtained for the OMZ agree with previous estimates (eg. Correia and Ramalho, 1999). Calculated Moho temperatures cluster around 550-590 °C. Best-fitting heat production values (in the sense that the values can reproduce the average geotherm) are 1.8, 0.8, and 0.3 $\mu\text{W m}^{-3}$ in the three crustal layers. These values are consistent with measured upper crustal values in the OMZ and average crustal compositions in various tectonic settings. In the SPZ, acceptable Moho temperatures (590-630 °C), together with Moho heat flow restricted to less than 30 mW m^{-2} , require a highly radioactive upper crust. Best-fitting (in the sense defined above) heat production values in the three crustal layers are 3.3, 0.7, and 0.3 $\mu\text{W m}^{-3}$, respectively.

From these results, it can be concluded that the difference in surface heat flow between the Ossa-Morena and South Portuguese Zones can be attributed to differences in heat production values in a felsic upper crustal layer. The SPZ is generally about 30-40 °C hotter than the OMZ at the base of the crust (refer to Table 4.3). This temperature difference is not significant as it lies within the 2σ errors calculated for each zone. The geotherms produced in this thesis for the OMZ and the SPZ diverge to a maximum at the base of the upper crust and then converge towards the base of the lithosphere. This differs from previous work

where the geotherms in the two zones diverge throughout the crust. Differences in the heat flow component from beneath the crust for the two zones are smaller than $1\text{--}2\text{ mW m}^{-2}$, which is well within the 2σ errors assigned to the calculated values of q_M . This is to be expected because of the geographic proximity of the OMZ and the SPZ. Since the two zones are of similar tectonic age and structure, it is more realistic to ascribe differences in surface heat flow to variations in the upper crust than to differences in sub-crustal heat flow. The average Moho heat flow calculated for the OMZ and SPZ in Southern Portugal is $26.8 \pm 4.4\text{ mW m}^{-2}$. This result helps to substantiate the argument that there is a direct relationship between Moho heat flow and the age of tectonic provinces. Accepted Moho heat flow values are usually in the range of $12\text{--}16\text{ mW m}^{-2}$ for Precambrian shields and around $20\text{--}30\text{ mW m}^{-2}$ in Paleozoic settings (Čermák et al., 1991). It has been somewhat accepted that on average, continental surface heat flow can be partitioned into two main sources with about 40% of the heat flow contribution coming from radioactive heat production in the crust and the remaining 60% coming from sub-crustal heat flow (eg. Pollack and Chapman, 1977). This partition does not hold true for the OMZ and SPZ, as the sub-crustal heat flow (q_M) is less than 50% of the surface heat flow. This would suggest that either crustal heat production in this region is anomalously high, or that perhaps the partitioning of heat flow sources should be re-examined.

7.2 Discussion of rheological results and comparison with other tectonic provinces

The rheological results presented in chapter 6 show that the lithosphere of the Ossa-Morena and South Portuguese Zones is horizontally stratified into brittle and ductile layers (see Figs. 6.1-6.4). Although there is a large amount of uncertainty associated with creep parameters, rheological profiles are accurate as a first approximation. Rheologically weak layers, present at the base of the upper, middle, and lower crust under hydrostatic conditions ($\lambda = 0.4$) thin or disappear under nearly lithostatic conditions ($\lambda = 0.9$). The two-dimensional rheological profiles (Figs. 6.5-6.8) show that the majority of weak ductile layers are continuous between the two zones. Rheological stratification of the lithosphere has important geodynamic consequences. Due to the presence of weak layers, the mechanical behaviour of the lithosphere is not the same under lateral loading as under vertical loading: the soft layers can act as decoupling horizons, resulting in large-scale overthrusting and intralithospheric décollements (Ranalli, 1995). The total lithospheric strength is estimated at 10^{12} - 10^{13} N m⁻¹ for both zones. This is within the usual range for continental lithosphere (Ranalli, 1991).

7.3 Comparison of lithospheric thickness

Estimates of the thickness of the lithosphere were made for both a thermal lithosphere where the lower boundary is defined in terms of the melting

temperature of peridotite and for a rheological lithosphere where the lower boundary is defined by the minimum critical strength of a 'rigid' lithospheric plate. Fernández et al. (1998) found that the lithospheric thickness of the Iberian Massif, constrained by heat flow, heat production, and surface elevation data, seems to remain almost constant at around 110 ± 5 km. More specifically, they concluded that for the southern part of the massif, the thermal lithospheric thickness is 107 – 112 km. This estimate is lower than the thickness of the thermal lithosphere calculated in section 4.8 (121 – 143 km for the Ossa-Morena Zone and 118 – 141 km for the South Portuguese Zone). This difference can be mainly attributed to the use of hotter geotherms in the estimate given by Fernández et al. (1998). A thinner thermal lithosphere is expected in the SPZ to coincide with the higher observed surface heat flow for this zone. The difference, however, is hardly significant. As shown in Table 4.5, the thermal lithosphere of the SPZ is generally estimated to be 2-3 km thinner than that of the OMZ. This difference is within uncertainties associated with the estimates. Therefore, the thickness of the thermal lithosphere for both the OMZ and the SPZ obtained in this thesis is about 120 – 140 km. In section 6.4, the rheological lithosphere is estimated to be 103 – 116 km in the Ossa-Morena Zone and 100 – 113 km in the South Portuguese Zone. Again, differences in the thickness of the lithosphere between the two zones are not significant given the relative uncertainties. The rheological lithosphere for the two zones is estimated to be approximately 100 – 115 km thick if the lower limit of the lithosphere is at $\sigma = 1$ MPa, and about 20

km thinner if the lower limit is at $\sigma = 10$ MPa. These values are within the expected range for Paleozoic massifs (e.g. Ranalli, 1995).

7.4 Ambiguity of the geothermal problem

If only surface heat flow values can be used in the testing of geothermal models, there will always be an indefinite number of heat production rate and thermal conductivity value combinations that yield the measured surface heat flow. By the same token, this means that forward thermal modelling of the lithosphere is easy, because a single acceptable parameter combination is quickly found, but the real representivity of such results is much more difficult to judge (Jokinen and Kukkonen, 1999). By use of a DSPS method, this ambiguity is partly compensated for by the inclusion of multiple possible solutions. The full ranges of parameters considered using this method are summarized in Table 4.2. In order to decrease the number of potential combinations of thermal conductivity and heat production rate that produce the desired value of surface heat flow, more information must be brought to the system.

It is important to note that relatively large variations in the geotherm can result from changes in values of heat production and thermal conductivity. An average crustal value of $K = 2.5 \text{ W m}^{-1}\text{K}^{-1}$ (eg. Clauser and Huenges, 1995; Mareschal et al., 2000) is often assumed for geothermal studies, with no real regard for rock

type or variations in pressure and temperature with depth. This assumption can introduce a large amount of uncertainty into the equation. Numerical results obtained from typical representative values of heat production and thermal conductivity are not necessarily invalid; however, they should be taken as approximate values and the inherent uncertainty should always be considered. The methods developed in this thesis can provide a useful option for similar geothermal studies in areas where heat flow data is scarce.

7.5 Future work

Further work in this region would help to clarify the geothermal problem. More detailed surface heat flow surveys and more extensive heat production measurements would aid in the production of more accurate regional geotherms. Better constraints on the temperature profile would in turn lead to a more complete understanding of the rheological properties of the lithosphere as well as improved estimates of thermal and rheological lithospheric thickness. Studying the lithospheric structure can help advance the understanding of its long-term evolution (Čermák, 1982). Detailed geothermal studies of the Iberian Massif in Southern Portugal can help to provide a better understanding of the thermal and rheological state of the crust in related Variscan Massifs and similar tectonic regions.

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