# Estimation of heat flow and geothermal gradient from numerical modelling in central Portugal

A.J.S.C. Pereira[1], J.J. Costa[2], M. Panão[2], M.M. Miranda[1,3], A. Machadinho[4], R. Lamas[1], L.J.P.F. Neves[1], N.V. Rodrigues[1]

[1] CEMUC/ Department of Earth Sciences, University of Coimbra, Rua Sílvio Lima, Polo II, 3030-790 Coimbra

[2] ADAI-LAETA/ Department of Mechanical Engineering, University of Coimbra, Rua Luís Reis Santos, 3030-788 Coimbra

[3] IMAR, Department of Earth Sciences, University of Coimbra, Rua Sílvio Lima, Polo II, 3030-790 Coimbra

[4] Geosciences Center, Department of Earth Sciences, University of Coimbra, Rua Sílvio Lima, Polo II, 3030-790 Coimbra

mfldmiranda@gmail.com

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## ABSTRACT

Numerical modelling of heat flow and geothermal gradient is a useful tool in the absence of accurate measurements of such parameters when thermal conductivity and radiogenic heat production are known. This work describes a 2D thermal model that simulates the crust thermal state in Central Portugal aiming geothermal applications and more specifically EGS projects. This study focuses on granitic rocks, namely HHP granites, where estimated surface heat flows reach values in the range of 114 to 130 mW/m$^2$. In addition, the surface heat flow on a metasedimentary cover with various thicknesses was modelled to check its behaviour as a thermal blanket. The surface heat flow values are on the interval 100 to 115 mW/m$^2$. Both surface heat flow values for granites and metasediments are higher than mean published data. The depth for a possible EGS reservoir is predicted to be around 4 to 4.5 km in depth, where the temperature is estimated to reach 150 ºC.

## 1. INTRODUCTION

Amongst renewable energy options, geothermal energy has many attractive qualities stemming from the possibility of producing low-carbon base-load power and heat at a relatively low cost. Emerging technologies such as the Hot Dry Rock/ Enhanced Geothermal Systems (HDR/EGS) can greatly increase the worldwide geothermal potential provided that present-day technological limitations are overcome. Due to the considerable technical challenges and associated costs linked with those systems they can only to be considered if the geothermal resource has the potential to generate large quantities of electricity for a number of decades.

The central region of Mainland Portugal seems to have a significant potential for geothermal energy applications. This is supported by its large outcrops of Hercynian granitic rocks (tens of kilometres across) with considerable thickness (average and maximum thickness estimates of 5 km and 11 km; Machadinho 2014) in which occur several thermal springs with temperatures in the range of 20 ºC to 80 ºC (IGM 1998). Also the majority of the granitic rocks have high concentrations of radiogenic heat-producing elements U and Th (Godinho et al 1991; Lamas et al 2015b) and, consequently, high radiogenic heat production (RHP) rates (> 3.5 µW/m$^3$; Godinho et al 1991; Miranda et al 2015b).

This work aims at developing a 2D thermal model to estimate the heat flow and the geothermal gradient in a selected granitic pluton outcropping in Central Portugal. In the absence of accurate heat flow and geothermal gradient measurements, the numerical simulators using thermal conductivity and radiogenic heat production data from target area rocks are useful tools as a first approach for the assessment of the geothermal potential of an area of interest.

The numerical model described in this work allows to estimate the surface heat flow, the heat flow and temperature-at-depth curves, and it enables to predict the depth of a geothermal reservoir.

## 2. GEOLOGICAL FRAMEWORK

The estimations of heat flow and geothermal gradient were carried out in a segment 100 km wide of the Iberian Massif, covering 70 km of an outcropping granitic rock mass and 30 km of outcropping schists (Fig. 1). The lithology of interest in this study are the granitic rocks. Nevertheless, the segment is extended to include the schists as a way of simulating the influence of a metasedimentary cover in the surface heat flow and temperature field.

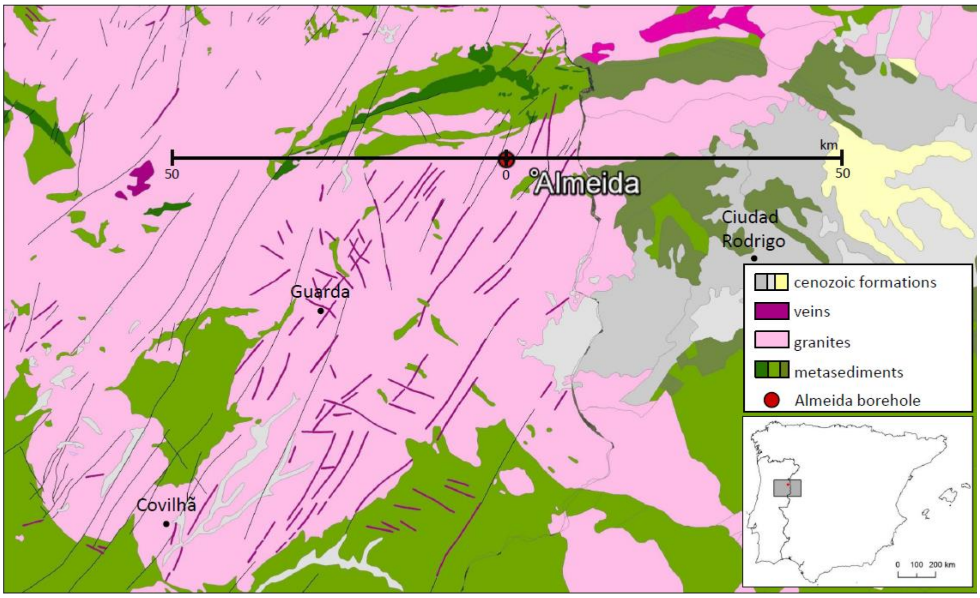


**Figure 1: Geological and geographical framework of the studied area. The black-line represents the studied segment.**

The granitic rock studied is locally known as Beiras Granitic Batholith and it is associated to the Hercynian plutonism in the Iberia authochthon. These granites were emplaced into a metasedimentary sequence (Schist-Greywacke Complex) of Proterozoic-Cambrian to Upper Carboniferous age, variably affected by the Hercynian deformation phases. The majority of the granitic rocks in the studied area are correlated to the last Hercynian phase (D3). This granitic suite was emplaced between 310-290 Ma (U-Pb zircon and monazite ages) and it is attributed to the late- to post-D3 group (Azevedo and Aguado 2013).

A borehole of about 1000 meters, with a core recovery of about 700 meters, was drilled in that granitic pluton near Almeida (Guarda; Fig. 1), and it was used as the central point of the segment modelled. From the borehole cores it is visible that, spite some local textural differentiations, the granitic mass is homogeneous in all its extension. According to Carvalhosa (1959) and Teixeira et al (1959), the batholith studied is a two-mica, but with prevalence of biotite, porphyritic granite with medium- to coarse-grain, with feldspar megacrystals. It is leucocratic with a grey colour when fresh/ non-altered, assuming a reddish tone in zones with metasomatic/ hydrothermal alteration. A more detailed description of the cores recovered from the borehole is given by Cortez (2013, unpublished) and a summary can be read in Miranda (2014). Due to the mineralogical content and high percentage of calco-sodic feldspars of the granitic rock it can be classified as a monzonitic granite (Carvalhosa 1959; Teixeira et al., 1959; Cortez, 2013, unpublished).

## 3. MATHEMATICAL MODEL AND NUMERICAL SOLUTION

The 2D thermal model has been developed in MATLAB to simulate the present-day in-depth temperature and heat flow distribution in the segment displayed in Figure 1. The approach is based on the numerical solution of the 2D steady-state heat conduction equation:

$$\partial/\partial x\ (k\ \partial T/\partial x) + \partial/\partial z\ (k\ \partial T/\partial z) + q'' = 0 \qquad [1]$$

over a rectangular domain of 100 km wide and 32 km deep, allowing for heterogeneous heat sources (q’’) and thermal conductivity (k) that may also vary with temperature. A uniform Moho heat flux of 25 $mW/m^2$ is assumed to be entering the domain through the lower horizontal boundary and the top boundary is considered to be at a constant and uniform surface temperature of 16 ºC. The vertical boundaries are both assumed adiabatic. The model is versatile enough to consider any number of different rock layers or masses, simply by specifying their geometry and thermal parameters. In each sub-domain, both the thermal conductivity and the rates of radiogenic heat generation can be specified with uniform values or as functions of depth or temperature.

The partial differential equation is integrated using finite-volume method described in Patankar (1980), where the calculation domain is discretized into a set of elementary control-volumes (CV), each one identified by a node. The values of the thermal conductivity at the CV interfaces are interpolated by the harmonic mean of the nodal values, in order to consistently handle step changes in material properties or in the heat generation rate. The resulting set of linear algebraic equations is solved by a tri-diagonal matrix algorithm. Calculations are performed with a uniform 400 m x 400 m grid, which has been shown to provide grid-independent results when compared with a 100 m x 100 m one. The criteria for convergence of the iterative procedure are: (i) normalized sum of the absolute residuals of all discretized equations $\leq 10^{-6}$; (ii) and maximum normalized iterative change of temperature $\leq 10^{-6}$.

## 4. INPUTS OF THE 2D THERMAL MODEL

The development of the 2D thermal model requires some information concerning the model's geometry which is given by geophysical and geological data and the thermal parameters of each model layer. Those inputs are discussed in the following sections.

### 4.1 Geophysical and geological data

Geophysical methods have been used to infer the granitic batholith's geometry and its relation with the crustal structure. The depth of the granite's root, as well as the continental crust structure, was deduced from geophysical data available for the Iberian Massif, namely gravimetric and magnetic data (Machadinho 2014) and seismic data (e.g., Banda et al 1981; Díaz and Gallart 2009). Data interpretation shows that the continental crust in the study area (Fig. 1) is 32 km deep, which is where the Moho discontinuity is reached. The continental crust structure used in our model consists of three main layers, whose depth and seismic velocity are described below:

1 – an upper crystalline layer with total thickness between 10 and 11 km, including a low-velocity layer. The top layer is 7 to 8 km thick and is characterized by a P-wave velocity ($v_p$) in the range of 5.9 – 6.1 km/s and the bottom lower-velocity layer has 3 to 4 km thick and $v_p$ of 5.6 km/s;

2 – a middle crust with thickness of 12 to 13 km and P-wave velocities of 6.2 – 6.3 km/s;

3 – a lower crust with 8 to 9 km thick and $v_p$ = 6.7 – 6.8 km/s.

To simulate the effect of a thermal cover on surface heat flow, the segment is laterally extended to include other country rocks (metasediments and cenozoic formations; Fig. 1). The main differences in the model's geometry are in the upper crystalline crust. That layer is subdivided into two sub-layers: one of country rocks superimposed to the crystalline continental crust.

The composition of the outcropping crystalline continental crust in the study area corresponds to granitic rocks and a metasedimentary sequence, based on published geological maps of Portugal and Iberia.

The low-velocity layer underlying the crystalline continental crust has been imaged from seismic data, not only in the Iberian Massif (e.g., Banda et al 1981, 1983; Díaz and Gallart 2009), but also in other places such as, for instance, in the Cornubian Batholith (e.g., Brooks et al 1984; LeBoutillier 2002 and references therein). Its top depth has been also detected by gravity and magnetic modelling and it has been interpreted as the granites lower contact with host rock. Near the studied area the inversion models reveal that this layer as an average depth of 7 km (Machadinho 2014). Despite a few attempts to explain the geological significance of this low-velocity layer, its discussion remains unresolved. However, several possible causes have been proposed: an internal granite boundary, a thrusting zone through granite or a large stopped block within granite pluton (Brooks et al 1984); geochemical mixing or granite compositional inhomogeneity (Finlayson et al 1979); a xenoliths accumulation zone (Bromley and Hall 1986); a brittle-ductile transition zone (Jones 1991); migmatites, mafic or residual cumulates layer at the base of granites (Lynn et al 1981). Another relevant aspect is that beneath a determinate depth there may be a slight P-wave velocity inversion if the rock composition is uniform with depth. Birch (1960, 1961) has measured the velocity of compressional waves at pressure to 10 kilobars and room temperature for several rock types. The author found that $v_p$ in granites increases with depth to a pressure corresponding to about 3 km depth as the pores collapse. Then the effect of the temperature increase overcomes the pressure increase causing a decrease with depth of $v_p$ (Holder and Bott 1971).

The composition of the middle and lower crust must be inferred by indirect methods and the deep crust nature is discussed in detail by various authors. Rudnick and Gao (2003, and references therein) present several proposals for the composition of the continental crust. In most of the proposals the middle and lower crust are considered to be composed of low- to medium-grade and high-grade metamorphic rocks, respectively. Those authors mention that for paleo-orogenic belts, as the Variscan belt, granulite-facies and eclogite-facies rocks may be important constituents of the middle and lower crust. Villaseca et al (1999) present a proposal for the nature and composition of the lower continental crust in Central Spain supported by geophysical data (Banda et al 1981) and by the granulitic xenolith suite study. The author suggests a felsic character for the lower continental crust being composed by felsic or politic granulitic rocks.

In the present work, a lower continental crust with a felsic character is assumed, as well as a middle crust composed of meta-igneous rocks.

### 4.2 Thermal parameters

The temperature-at-depth variations in the crust are controlled by several parameters such as surface temperature, basal heat flow, thermal conductivity of rocks, and the vertical distribution of radiogenic heat-producing elements U, Th and K (e.g., Casini 2012). The surface temperature of the target area is about 16ºC and the basal heat flow is assumed to be of 25mW/m$^2$, the remaining parameters are discussed below.

#### 4.2.1 Upper continental crust

Measurements on granite's thermal properties were carried out using the borehole that was drilled in the studied area (Miranda 2014; Miranda et al 2015a). Those rocks show an average thermal conductivity of 3.1 W/m/K which are in the range of values for this type of rocks (e.g., Wheildon et al 1980; Amaral et al 2013). It is well-known that thermal conductivity is a function of temperature and several empirical laws have been established to describe that behaviour (e.g., Lee and Deming 1998; Seipold 1998). To simplify the modelling, a constant value is used in each layer.

Since no thermal conductivity measurements were performed for metasedimentary cover, the value used is retrieved from literature relatively to schists from Portuguese territory (3.0 W/m/K; Correia 2015 and references therein).

Analysis on its radiogenic heat-producing elements from the granitic core of the borehole is also performed (Lamas et al 2015a; Neves et al 2015). The core-samples analysed show a U content of 14.3 ppm, a Th concentration of 17.5 ppm and 5.07 % of $K_2O$. Plotting the studied samples as a function of depth it is detectable a uniform vertical distribution of those elements, with no variation with depth, along the total borehole length. The RHP rate for the borehole is estimated using the following equation (Chiozzi et al 2002):

$$RHP = 10^{-5}\rho(9.51c_U + 2.56c_{Th} + 3.50c_K) \qquad [2]$$

where RHP is the radiogenic heat production rate (in $\mu W/m^3$) and $\rho$ is the rock density (in $kg/m^3$). The uranium and thorium concentrations ($c_U$ and $c_{Th}$) are in ppm, and potassium ($c_K$) is in %.

As for the radiogenic heat-producing elements, the RHP rate of the borehole has a uniform vertical trend distribution of the values (Lamas et al 2015a). On average, the borehole RHP is 5.2 $\mu W/m^3$, which is higher than the estimations carried out on fresh surface samples collected in the granitic batholith (RHP = 4.5 $\mu W/m^3$; Miranda et al 2015b). For the 2D thermal model presented in this work, the borehole RHP rate value was used as input for the model's granitic layer, as it is more representative of the RHP in depth.

Analysis of U, Th and K were carried out on samples of the Schist-Greywacke Complex outcropping in Central Portugal, and the RHP rate for those rocks has an average value of 1.6 $\mu W/m^3$.

As the lower-velocity layer in the base of the upper continental crust is still unresolved in terms of composition, one uses the empirical exponential law of Rybach (1976) and Rybach and Bunterbarth (1982, 1984) which is an attempt to assign realistic thermal parameters to deeper-seated layers of the crust that explains the RHP($v_p$) relationship – RHP decreases with increasing $v_p$:

$$\ln RHP = a - b\, v_p \qquad [2]$$

where RHP is the radiogenic heat production rate (in $\mu W/m^3$) and $v_p$ is the P-wave velocity (in km/s). The numerical factors a and b depend on pressure. For Precambrian rocks, and a pressure of 100 MPa, the numerical factors assume the values of 12.6 and 2.17, respectively (Rybach and Bunterbarth 1984).

The decrease in P-wave velocities within the crystalline continental crust reflects an increase of the radiogenic heat production rate of about 50 %. So, a granitic layer with a RHP rate of 5.2 $\mu W/m^3$ superimposed with an unknown material layer with 10.9 $\mu W/m^3$ is assumed for the modelling procedure. The thermal conductivity of this low-velocity layer is assumed to be of 2.5 W/m/K, as the value usually used in literature for the thermal conductivity of upper crust (Jiménez-Díaz et al 2012).

### 4.2.2 Middle and lower continental crust

The assumption of a middle crust with meta-igneous composition is based on literature, as explained in the above sections, and its RHP rate is estimated based on analysis of U, Th and K of that type of rocks. The average value obtained is 1.4 $\mu W/m^3$ and it was used as an input for the 2D thermal model.

For the lower continental crust, the RHP value for granulitic-facies rocks of Villaseca et al (1999, 2005) is used – 0.8 $\mu W/m^3$ to 0.96 $\mu W/m^3$.

Based on Jiménez-Díaz et al (2012 and references therein) the thermal conductivity for middle crust is assumed to be 2.5 W/m/K, and 2.1 W/m/K for lower crust. The geometry of the model ends up when reaches Moho layer which has as thermal parameters the values of 0.02 $\mu W/m^3$ for RHP rate (Jiménez-Díaz et al 2012 and references therein) and 3.0 W/m/K for thermal conductivity (Stüwe 2007).

## 5. RESULTS

The available dataset allowed the establishment of a conceptual thermal model for the crustal segment studied. To keep the modelling procedure as simple as possible, this thermal model uses a constant thermal conductivity and uniform RHP values for each layer. As the depths/ thicknesses of each crustal layer may vary (see section 4.1) several sensitivity studies were performed on the model. In those simulations some model geometries were tested to check the variability induced by the layers' depth on surface heat flow and temperature field. Table 1 shows the different geometries of each crustal layer applied on the model and the respective geothermal gradient and surface heat flow. For all the simulations the Moho is located at 32 km depth and the thermal parameters were kept constant. The results in Table 1 are related to the part of the crustal segment studied that only covers the granitic rocks, not taking into account the effect of the metasedimentary rocks (see Fig. 1).

As shown in Table 1, if the thicknesses of layers vary, it imposes some variability on the surface heat flow (q'') and on the geothermal gradient (dT/dz) will vary. The surface heat flow varies from 114 $mW/m^2$ to 130$mW/m^2$, and the geothermal gradient has values ranging from 32.5 K/m to 37.3 K/m. The higher heat flow and geothermal gradient results are linked with a thicker low-velocity highly productive layer (upper crust II).

**Table 1: Models' geometries used in the simulations to verify the differences induced on heat flow and geothermal gradient.**

| | dT/dz [K/m] | q'' [mW/m$^2$] | | Upper crust I [km] | Upper crust II [km] | Middle crust [km] | Lower crust [km] |
|---|---|---|---|---|---|---|---|
| | 32.46 | 114.4 | | 8 | 2 | 13 | 9 |
| | 34.64 | 121.1 | | 7 | 3 | 13 | 9 |
| | 37.09 | 128.8 | | 7 | 4 | 12 | 9 |
| | 37.32 | 129.5 | | 7 | 4 | 13 | 8 |
| | 34.92 | 122.0 | | 8 | 3 | 12 | 9 |
| | 35.15 | 122.7 | | 8 | 3 | 13 | 8 |
| Average | 35.26 | 123.1 | Mean | 7.5 | 3.2 | 12.7 | 8.7 |
| Error (95% CI) | 4.05% | 3.60% | Variability ± | 7.30% | 23.77% | 4.08% | 5.96% |

Due to the uncertainty of the layers' thicknesses and the variability that it induces in the results, the numerical modelling is carried out based on the thicknesses average values, except for the schist layer as it is illustrated in Figure 2.

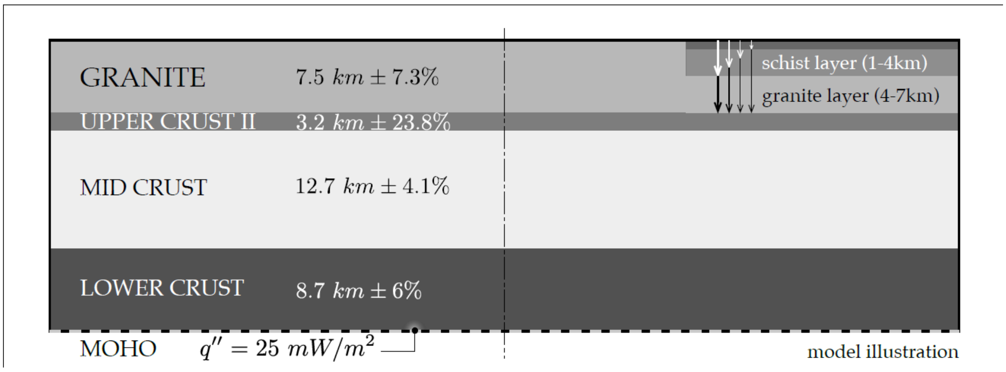


**Figure 2: Model illustration displaying the thicknesses used in the numerical modelling.**

To study the effect of the metasedimentary cover on heat flow and temperature field, due to the variability thickness, the schist layer is assumed to vary within an interval of 1 km to 4 km (Fig. 2). The influence of the thickness of schists on heat flow and temperature distribution as functions of depth is plotted in Figures 3 and 4, respectively. The profiles analysed are restricted to the 6 km depth because this is the maximum acceptable depth for a commercially viable EGS project. As displayed in Figure 3, the thicker the schist cover is more the surface heat flow decreases. This occurs due to a lower RHP rate of schists (1.4µW/m$^3$) when compared to the granites (5.2µW/m$^3$). As for heat flow, the temperature-at-depth curve also decreases as the schists thickness increases (Fig. 4).

In the granitic rocks domain of the segment studied (see Fig. 1), the surface heat flow reaches a value of ~ 120 mW/m$^2$ (Table 1; Fig. 3). If a schist layer is superimposed to the granites, the surface heat flow decreases and, depending on the layer thickness, it can vary from ~ 115 mW/m$^2$ (for 1 km of schist) to ~ 100mW/m$^2$ (for schists with 4 km thick).

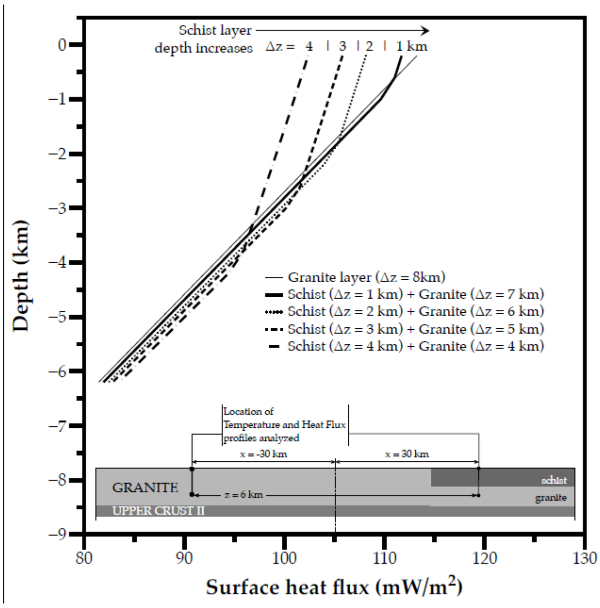


**Figure 3: Heat flow variation induced by the metasedimentary cover thickness.**

As Figure 4 shows at 6 km deep, the granite curve reaches a temperature of 210 ºC, while for the schists + granites profile the temperatures ranges between ~ 205 ºC (for schist having 1 km thick) to ~ 185 ºC (for the maximum schists thickness assumed).

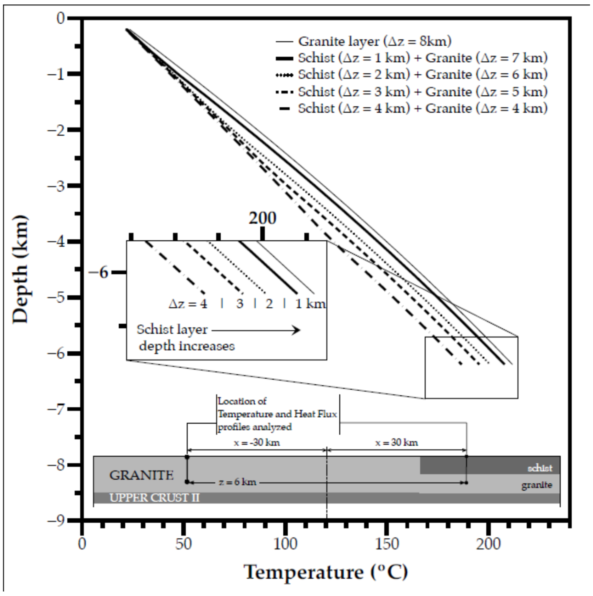


**Figure 4: Temperature profiles for the different schists thicknesses.**

Given the obtained results in terms of surface heat flow and temperature-at-depth, the schist layer is assumed to have a maximum of 2 km thick. Thus, the thermal modelling results would not be overestimated or underestimated.

## 6. DISCUSSION AND CONCLUSION

As mentioned in the previous section, the RHP rate is assumed to have a constant value for each layer. The assumption of a uniform value for each layer and not one that follows an exponential law (Singh and Negi 1980) is justifiable by the remarkably uniform distribution of RHP rate along the total length of the deep borehole drilled in the studied area (Lamas et al 2015a). This uniform distribution in depth of RHP rate for granites was also detected in those of SW England as Sams and Thomas-Betts (1988 and references therein) referred in their paper.

The modelling carried out for the surface heat flow along the crustal segment selected (see Fig. 1) exhibit some variability (100 mW/m$^2$ and 120 mW/m$^2$; Table 1; Fig. 3) but still higher values than the published average estimations for Iberia (65 mW/m$^2$ to 73mW/m$^2$; e.g., Banda et al 1991; Fernàndez et al 1998; Tejero and Ruiz 2002; Jiménez-Díaz et al 2012; Chamorro et al 2014) often used for thermal modelling purposes and on studies of the geothermal potential. This highlights that using average literature values for geothermal calculations can lead to significant errors in the analysis of the geothermal regime of a region.

The surface heat flow estimations (Fig. 3) for the granites are in the range of values referred in literature for the Cornubian Batholith (Cornwall, SW England). For those granitic rocks the heat flow interval is between 110 mW/m$^2$ to 120 mW/m$^2$ (e.g., Webb et al 1985, 1987). Those values are due to their high concentrations on heat-producing elements. For example, the Carnmenellis granite has in average 10.8 ppm of U, 17.2 ppm of Th, and 4.28 % of K (Tammemagi and Smith 1975), which are nearly the concentrations obtained on both the deep borehole (Lamas et al 2015a; Neves et al 2015) and on surface samples (Lamas et al 2015b; Miranda et al 2015b) of the Beiras Granitic Batholith.

For an EGS project it has generally been considered that the geothermal reservoir is required to have a temperature of at least 150 ºC and has to be at a lower depth than 5 km for the project to be commercially viable (e.g., Gillespie et al 2013). From the temperature fields estimations (Fig. 4), the 150 ºC is reached at depths of 4 km (for the granite layer curve) and 4.5 km (for 2 km thick schist layer superimposed to granites). Those depths are within the widely quoted practical lower limit for exploiting EGS resources.

The thermal modelling results also point out to temperatures around 600 ºC for the Moho, which are within the temperature interval mentioned by other authors (600 ºC – 700 ºC; Jiménez-Díaz et al 2012; Machadinho et al 2014).

As data concerning heat flow measurements in shallow wells are absent in the selected crustal segment studied, the temperature results from the developed 2D thermal model were compared with the water temperature measured in the Almeida’s deep borehole (see Fig. 1), assuming the system is in thermal equilibrium. The thermal water exploited in this well reaches the surface at a temperature of 17 ºC (Ferreira Gomes et al 2015). At a depth of 500 meters, the author mentions that the water temperature is 30 ºC. In the developed model, at that depth the temperature estimation matches the 30 ºC, which means that the estimations of heat flow and geothermal gradient carried out in this work are accurate approximations of the real situation.

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