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A MATLAB-derived software (geothermMOD1.2) for one-dimensional thermal modeling, and its application to the Corsica-Sardinia batholith

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ABSTRACT

Determination of the thermal state of the crust is of fundamental importance to understand the feedbacks between tectonics, rheology and metamorphism. The most important parameters controlling the variation of temperature with depth in the crust are the heat flow across the Moho, the thermal conductivity and the vertical distribution of heat-producing elements $^{238,235}U$, ^{232}Th and ^{40}K. The Corsica-Sardinia batholith formed during a regional high-temperature metamorphic event by extensive partial melting of the Variscan crust. Petrologic observations indicate that most granites and migmatites formed between 0.6–0.2 GPa, requiring the geotherms to flatten substantially relative to the stage of crustal thickening. The adjustment of geotherms may be interpreted in terms of enrichment in heat-producing elements or, alternatively, in terms of increased mantle contribution. The validity of these two end-member hypothesis has been tested by performing numerical experiments with a software package appositely developed in Matlab. The software allows to set up crustal model composed of up to five different layers, and to plot the calculated geotherm along with the stability field of the haplogranite system and other thermo-barometric constraints. The steady-state thermal structure of the Sardinian Variscan crust has been computed at four different time steps (320, 310, 300, and 280 Ma), which cover the batholith evolution. The geometry and composition of each of these crustal models has been constrained based on geophysical observations, geochronology and petrology. In a first experiment, the heat conduction equation has been solved for all of the four time-steps, assuming constant (15 mW/m^2) heat flow across the Moho in order to simulate a 'fully crustal' evolution of the thermal structure. The alternative has been simulated in a second experiment, by rising the basal heat flow up to 40 mW/m^2 during the last two time steps.

1. Introduction

The thermal state of the Earth's crust controls various processes, such as the deformational behavior of rocks, metamorphism, and anatexis; thus, it is fundamental to addressing a range of geological disciplines as disparate as geodynamics, petrology, and seismology. Temperature variations in the crust are influenced mainly by surface temperature, basal heat flow, the specific thermal conductivity of rocks, and the vertical distribution of radiogenic heat-producing elements such as $^{238,235}U$, hereafter indicated collectively as U, ^{232}Th, and ^{40}K. Although several of these variables can be determined to within experimental errors, there are major uncertainties in the vertical distribution of heat-producing elements due to limited information on the geometry and composition of the crust.

This shortcoming imposes severe limitations on the resolution of geothermal models, although this problem has been partly overcome (Srivastava et al., 2009) using a stochastic approach, which takes into account both the variability of thermal conductivity and the heterogeneous distribution of heat-producing elements in the crust. Application of this method requires that at least two boundary conditions are known, such as the surface temperature and the surface heat flow. Because both of these parameters can be measured directly in the field, the actual geotherm of a given region can be quickly evaluated. However, to accurately constrain the thermal structure and thermal evolution of past collisional belts would require the development of crustal models with appropriate values for the relevant variables, because neither of the above boundary conditions can be measured directly in exhumed mountain chains. On the other hand, exhumed chains may provide access to almost complete crustal sections, from the sedimentary layer to the lower crust; as such, the geometry of the Earth's interior can be accurately constrained, and rock-specific parameters can be measured directly with a high degree of accuracy.

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This paper presents a MATLAB-derived software (geothermMOD1.2) devoted to one-dimensional thermal modeling. The program is intended as a tool for designing any type of crustal model, running numerical experiments, and evaluating the consistency of results by comparing them with independent thermobarometric constraints. The package consists of an "m-file" integrated with a simple graphical user interface (GUI), both developed in Matlab (version r2010a). The user can build their own crustal models by entering the following parameters directly into editable fields in the GUI: abundances of the heat-producing elements (U, ^{232}Th, and ^{40}K), average thermal conductivity, mean density, and crustal thickness. By allowing the user to construct models comprising up to five different layers, each with its own specific input parameters, maximum design flexibility is ensured. In addition, users can modify the remaining variables of the heat equation (i.e., basal heat flow and the surface temperature) as required. Of interest to users devoted to the reconstruction of ancient thermal structures, the software considers the decay of heat-producing elements, enabling calculation of the abundances of *U*, ^{232}Th, and ^{40}K at the model age at which the geotherm is to be evaluated. Finally, users can check the consistency of calculated thermal structures by appending their own thermo-barometric constraints to the plot, or by adding the solidus/liquidus curves for haplogranite systems or the aluminosilicate stability fields. The curves made available for plotting are based on the nature of the demonstration dataset, and can be readily replaced or augmented by other petrologic constraints, as the software is not compiled and can therefore be customized.

2. Mathematical arguments

2.1. Heat conduction equation

In one dimension, the governing equation for heat conduction involving a component of radiogenic heat production is

$$\partial T/\partial t = \kappa \partial^2 T/C_p \rho \partial z^2 + A/C_p \rho \quad (1)$$

where T is temperature (°C), t is time (s), κ is thermal conductivity (Wm^{-1} °C^{-1}), C_p is specific heat (Jkg^{-1} °C^{-1}), ρ is density (kgm^{-3}), z is depth (m), and the term A represents the volumetric heat production rate (Wm^{-3}). An average value for thermal conductivity is arbitrarily assigned to each layer, and although some temperature-dependence can be expected (Vosteen and Schellschmidt, 2003; Wittington et al., 2009) the errors associated with this analytical simplification can be minimized by entering appropriate values for layers of different composition. For a geotherm in equilibrium, temperature will not vary with time, meaning that the first term of (1) will be equal to zero and that the heat equation at steady state can be simplified to

$$\partial^2 T/\partial z^2 = -A/\kappa \quad (2)$$

Eq. (2) is a second-order partial differential equation; thus, at least two boundary conditions are required to find a solution. A pair of boundary conditions is conveniently provided by setting the temperature at $z=0$ to T_0 (surface temperature) and the heat flow at $z=0$ to Q_0 (surface heat flow). The immediate advantage of this choice is that both boundary conditions are easily measurable in the field. By integrating Eq. (2) and using the above boundary conditions to constrain the integration constants, the heat equation can be solved as follows:

$$\partial T/\partial z = -A/\kappa + c_1 \quad (3)$$

$$c_1 = Q_0/\kappa \quad (4)$$

Integrating once again, we have

$$\partial T/\partial z = -A/\kappa + Q_0/\kappa + c_2 \quad (5)$$

$$c_2 = T_0 \quad (6)$$

$$T = -Az^2/2\kappa + Q_0 z/\kappa + T_0 \quad (7)$$

The solution of Eq. (7) for the specified set of boundary conditions represents the temperature at the base of a layer of finite thickness z, characterized by a volumetric heat production rate of A and a basal heat flow $Q_b = Q_0 - Az$.

2.2. Heat-production rates in the past

Heat production in the crust is fundamentally related to the radioactive decay of numerous isotopes, but only U, ^{232}Th, and ^{40}K contribute significantly to the thermal budget, as described by the following equation (Rybach, 1988):

$$H = \rho[(9.52cU) + (2.56cTh) + (3.48cK)] \times 10^{-5} \quad (8)$$

Using appropriate concentration for *c*U (ppm), *c*Th (ppm), and *c*K (%), and the averaged value of ρ, Eq. (8) yields the volumetric heat production rate (μWm^{-3}) of a given layer. Therefore, the actual heat production rate of a layer may be immediately calculated if its thickness and the volumetric abundance of radioactive isotopes are known; both of these variables can be realistically constrained in exhumed collisional chains in which complete crustal sections are exposed. Provided that the decay constants are independent of temperature and time, an appropriate data set permits calculation of the past heat-production rate of a given layer by back-calculating the past amount of any heat-producing element, as follows:

$$X_{i\ past} = [X_{i\,actual}/exp(\alpha_i t_p)]z \quad (9)$$

where $X_{i\ past}$ is the past abundance of the radioactive isotope i, $X_{i\ actual}$ is the actual abundance of the same isotope, the term α_i represents the relevant decay constant, z is the thickness of the layer containing the isotopes, and t_p is the age for which the isotopic content is to be recalculated.

3. Numerical modeling

3.1. Application to the Corsica-Sardinia batholith

The numerical solutions of Eq. (7), computed using the geothermMOD1.2 software, are used here to test two fundamentally different genetic models of the north Sardinian region of the Variscan Corsica-Sardinia batholith. This part of the batholith formed over a relatively long period, between approximately 320 and 280 Ma (Paquette et al., 2003; Gaggero et al., 2007; Oggiano et al., 2007), and the oldest granitic plutons appear to be related to anatexis of metamorphosed crust at amphibolite-facies depths (Macera et al., 2011). Field relationships, geochronology, and thermobarometry indicate that temperatures of at least 680–730 °C were reached at depths of 15–21 km (Giacomini et al., 2005; Cruciani et al., 2008), given the composition of anatectic melts. Once the required conditions for partial melting were reached, the thermal structure was maintained in the upper crust for ca. 40 Ma. The efficiency of partial melting increased with time, and shifted progressively toward shallower depths; this indicates the establishment of a high-heat-flow regime, a feature that is common to most other Variscan belts (Echtler and Malavieille, 1990; Lexa et al., 2011). The cause of such a high thermal gradient is a topic that remains controversial, in fact it might resulted from enrichment in heat-producing elements or from mantle upwelling (Cocherie et al., 1994; Faure et al., 2010). The applicability of either