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GEOTHERM: a finite difference code for testing metamorphic P–T–t paths and tectonic models

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Here, time-dependent solutions for the heat conduction equation are numerically evaluated in 1D space using a fully implicit algorithm based on the finite difference method, assuming temperature-dependence of thermal conductivity. The method is implemented using the package ‘GEOTHERM’, comprising 13 MATLAB-derived scripts and 3 Excel spreadsheets. In the package, the initial state of the modeled crust, including its thickness, average density, and average heat production rate, can be configured by the user. The exhumation/burial history and metamorphic evolution of the crust are simulated by changing these initial values to fit the vertical displacement rates of the crust imposed by the user. Once the inputs have been made, the variations with depth of temperature, proportion of melt, and shear stress, as well as average values of heat flow at the surface and across the Moho, are calculated and displayed in five separate plots. The code is demonstrated with respect to the Carboniferous evolution of the South Variscan Belt. The best fit to independent petrologic constraints derived from thermobarometry is obtained with an early Carboniferous (342 Ma) slab break-off and a shear strain rate of $10^{-13}$ s$^{-1}$ between 318 and 305 Ma.

1. Introduction

A major shortcoming of interpreting metamorphic pressure–temperature–time (P–T–t) paths obtained by interpolation of P–T conditions deduced from the composition of metamorphic mineral assemblages and geochronology is that mineral assemblages record at best only a few snapshots of the evolution of orogens. Therefore, the extrapolated geotherms cannot be linked to a specific tectonic setting in a simple way, and petrologic datasets, although robustly constrained, often give rise to contrasting interpretations (e.g., Lardeaux et al., 2001; Ledru et al., 2001; Giacomini et al.,
2006; Bellot and Roig, 2007; Duguet et al., 2007; Vilà et al., 2007; Cruciani et al., 2008; Faure et al., 2010; Langone et al., 2010). Additional uncertainty is introduced because diffusion rates of cations in minerals exhibit very different T–P–fH2O dependence (e.g., Cherniak and Watson, 2000; Farver and Yund, 2000) involving potentially large discrepancies between the inferred isotopic ages and metamorphic peak conditions (Burton and O’Nions, 1992). These observations imply that past geotherms and geodynamic models extrapolated directly from P–T–t paths are subject to considerable bias.

This paper presents a MATLAB-derived software package (GEOTHERM) devoted to the one-dimensional modeling of transient thermal structures. The program is intended as a user-friendly tool for designing any type of crustal model (in extension or shortening, or a combination of both), conducting numerical experiments, and evaluating the consistency of independent P–T–t constraints. GEOTHERM is derived from the code geothermMOD1.2 (Casini, 2012) and implements a fully implicit finite difference algorithm that solves the transient heat conduction equation subject to initial conditions and Dirichlet-type boundary conditions. Users can design lithospheric models composed of up to three distinct crustal layers, each with characteristic heat production rate and thickness. The initial thickness and heat production rate of the mantle lithosphere are instead given as pre-defined input parameters. Both radioactive heating \( H_r \) and shear heating \( H_s \) are incorporated into the heat equation and evaluated at each time-step based on the geodynamic evolution imposed by the user. Relevant physical parameters such as thermal conductivity \( \kappa \), specific heat capacity \( C_p \), and thermal diffusivity \( k \) are all formulated as functions of temperature (Vosteen and Schellschmidt, 2003; Wittington et al., 2009), so the code automatically adjusts the initial values as temperature changes with time across the crustal section. The effect of partial melting on the rheology and geometry of the model is implemented by dynamically adjusting the thickness, composition, and effective viscosity of the modeled layers in response to changing the melt-to-solid ratio across the modeled crust.

The package consists of 13 “m-files” developed in MATLAB (version r2010a) integrated with 3 spreadsheets (Microsoft Excel 1997–2003). The user can build his/her own crustal models by entering the following parameters directly into appropriate fields in the spreadsheet ‘data.xls’: i) bulk crustal thickness ([m]) at the beginning of the experiment \( t = t_0 \) and at the end \( t = t_{fin} \), as well as at any intermediate period \( t = t_n \); ii) volumetric heat production rate at time \( t = t_0 \) \( (H, \ [\mu W m^{-3}]) \), and iii) thickness of the layers (m) at time \( t = t_0 \). Optionally, the standard deviation of \( H \) (sdH, \( \ [\mu W m^{-3}] \)) can be specified to evaluate the errors derived from averaging large data base of heat production rates (Casini, 2012). Assuming that the exhumation/burial rates are independent of
temperature, the tectonic setting (either extensional, compressive, or a combination of both) is implemented by adjusting the bulk crustal thickness over time. Therefore, negative increments of bulk crustal thickness reflect uplift and erosion, whereas positive increments indicate shortening. Three different scenarios are permitted: i) lithosphere stability, ii) slab break-off, and iii) rise of a mantle plume. In each of these cases, the user is able to set up both the start and end times (in Ma) of the relevant geodynamic event to be simulated during the experiment. In addition, the user can optionally simulate the effect of up to 10 distinct shearing events, each with its own specific strain rate and duration. Finally, the user can interactively check the consistency of calculated thermal structures by comparing the relative error between simulated geotherms and the curve constructed at each time step from polynomial fitting of up to 100 different P–T–t constraints. Statistical accuracy is ensured by providing each petrologic constraint with its own specific standard deviation for temperature (K), pressure (GPa), and age (Ma). The results of numerical simulation are displayed as movies on the screen, saved automatically as ‘experiment.avi’ files and made available for use outside the MATLAB environment.

Here, the GEOTHERM package is tested with respect to the evolution of the South European Variscan Belt (Rossi et al., 2009), including an exploration of the possible relationship between slab break-off and high-temperature (HT) metamorphism at around the Carboniferous–Permian boundary (Giacomini et al., 2006; Casini and Oggiano, 2008; Faure et al., 2010). The results of the numerical simulation argue for slab break-off in the early Carboniferous and exclude it as a cause of the late Variscan HT event.

2. Theoretical approach

2.1 Governing equations

In one dimension, the governing equation for heat conduction with temperature-dependent thermal conductivity (Vosteen and Schellschmidt, 2003; Wittington et al., 2009) and heat sources is the second-order partial differential equation:

\[
\frac{\partial T}{\partial t} = \frac{1}{C_p \rho \kappa} \frac{\partial}{\partial z} \left( \kappa \frac{\partial T}{\partial z} \right) + \frac{H}{C_p \rho}
\]  

where \( T \) is temperature (K), \( t \) is time (s), \( \kappa \) is thermal conductivity (m\(^2\)s\(^{-1}\)), \( C_p \) is specific heat (Jkg\(^{-1}\)°C\(^{-1}\)), \( \rho \) is density (kgm\(^{-3}\)), \( z \) is depth(m), and the term \( H = (H_r + H_s) \) represents the volumetric heat production rate (Wm\(^{-3}\)) due to the decay of radioactive elements (\( H_r \)) and shear heating (\( H_s \)). The average volumetric heat production rate at time = \( t \) may be calculated from the \( ^{235,238}\)U, \( ^{232}\)Th, and \( ^{40}\)K composition of the modeled layers at time = \( t \), as follows (Rybach, 1988):
\[ H = \rho[(9.52 \ 235,238 U^c) + (2.56 \ 232 Th^i) + (3.48 \ 40 K^i)] \times 10^{-5} \]  

(2)

For a transient geotherm, temperature will generally vary with time in response to variations in bulk crustal thickness and the relative thickness and composition of the layers. This implies that partial derivatives in Eq. (1) should be approximated by finite difference expressions.

### 2.2 Finite difference approximation

The thermal structure of a modeled lithosphere is evaluated at 151 variably spaced nodes, where the first 101 nodes represent the lithosphere and the last 50 are regularly distributed from the lithosphere–asthenosphere boundary (LAB) to the bottom of the model which is taken as a constant depth of 1650 km. In all sets of numerical simulations, the depth of the lithosphere ranges from about 60 to 250 km, so the grid resolution varies between about 0.5 and 3.5 km, depending on the imposed boundary conditions. Equation (1) is solved at the grid points by using a fully implicit algorithm that implements specific heat, thermal conductivity, and diffusivity as temperature-dependent parameters. Partial derivatives in Eq. (1) are approximated as:

\[
\frac{\partial T}{\partial t} = \frac{(T_{j+1}^{n+1} - T_j^{n+1})}{\Delta t}  
\]

(3)

\[
\frac{\partial}{\partial z} (\kappa \frac{\partial T}{\partial z}) = \left[ \frac{\kappa_{j+1/2} (T_{j+1}^{n+1} - T_j^{n+1})}{\Delta z^2} - \frac{\kappa_{j-1/2} (T_{j+1}^{n+1} - T_j^{n+1})}{2 \Delta z^2} \right]  
\]

(4)

where subscripts denote the position of points along the 1D grid (Fig. 1), and superscripts denote the value dimension at the current \((n)\) and future time steps \((n+1)\). Substituting Eqs (3) and (4) into Eq. (1) gives the finite difference scheme:

\[
- S_k^{P, n} T_j^{n+1} + B T_j^{n+1} - S_k^{P, n-1} T_j^{n+1} = \frac{dt}{\rho C_p (H^P)} + T_j^P  
\]

(5)

where \(S = \Delta t/2\Delta z^2\) and \(B = 1 + S_k^{P, n+1/2} + S_k^{P, n-1/2}\). This system of linear equations may be conveniently written in matrix format as:

\[
[\text{A}] \begin{bmatrix} T_1^{n+1} \\ \vdots \\ T_{151}^{n+1} \end{bmatrix} = \begin{bmatrix} T_1^P \\ \vdots \\ T_{151}^P \end{bmatrix}  
\]

(6)

where the \(\text{A}\) matrix on the left-hand side of Eq. (6) stores the coefficients of terms in \(T^{n+1}\), the right-hand vector hosts the constants from the right-hand side of Eq. (5), and the solutions are contained...
in vector b. New temperatures (time $t = t^{n+1}$) are thus determined by solving Eq. (6) using Gaussian elimination at each time step.

### 2.3 Initial and boundary conditions

The application of finite difference methods requires that both initial and boundary conditions are available for Eq. (1) to be solved as a function of time. An initial temperature profile is derived from the steady-state solution of Eq. (1) at every node of the grid, using the specified initial thicknesses of layers and the average volumetric heat-production rate set by the user at time $= t_0$. Following the usual approach, a Dirichlet boundary condition is applied to the upper node; therefore, a constant temperature of 273.15 K is imposed at the surface ($T_{z=0} = T_{surf}$). For the lower boundary, both constant temperature and constant flux (Neumann) boundary conditions are usually applied (Casini, 2012). In this paper, the lower boundary of the model (1650 km) is placed far below the region of interest, and therefore a Dirichlet boundary condition should be conveniently applied, as differences in the lithospheric temperature distribution due to the application of one or the other type of lower boundary condition are minimal. Based on this, the lower node is maintained at a constant temperature of 2323.15 K, which yields a temperature of approximately 1573.15°C at 150 km depth in a stable crust, using a meaningful linear temperature gradient of 0.5 K km$^{-1}$ in the mantle.

### 2.4 Partial melting

Partial melting of the crust is an important process that provides strong feedback into the rheology, deformation, and compositional evolution of the lithosphere (Petford et al., 2000; Rosenberg and Handy, 2005; Schulmann et al., 2009). Therefore, GEOTHERM allows melting of crustal rocks in the section of the profile crossing the solidus/liquidus curves of crustal rocks. To a first approximation, the proportion of melt $\phi$ in crustal rocks is assumed to be independent of time and to increase linearly with $T$ as follows (e.g., Burg and Gerya, 2005):

$$
\begin{align*}
\phi &= 0 \quad &T < T_s \\
\phi &= \left( \frac{T - T_s}{T_l - T_s} \right) \quad &T_s < T < T_l \\
\phi &= 1 \quad &T > T_l
\end{align*}
$$

where $T_s$ and $T_l$ represent the solidus/liquidus curves of granite (Johannes and Holtz, 1996) and tonalite (Patiño Douce, 2005), respectively. The melt proportion (M) in the crust is evaluated based on the temperature distribution for the current time step.
The effect of upward melt migration on the evolution of the crust is simply implemented by assuming that melt cannot escape its source region until the melt-to-solid ratio reaches a critical value of $M = 0.06$ (e.g., Vogt et al., 2011). Once this value is exceeded, all melt above a non-extractable amount of $M_{\text{min}} = 0.02$ and below a threshold of $M_{\text{max}} = 0.35$ is extracted and flows almost instantaneously upward through channels or dykes (e.g., Petford et al., 2000), accumulating below the brittle–ductile transition. The ideal endothermic behavior of melt-producing reactions is approximated maintaining the nodes in the partially molten region at the melting temperature until the reactants are consumed. Assuming that melt is produced in layer 3, melt migration increases the bulk thickness of layer 2 while the thickness of layer 3 decreases proportionally. Yet, limiting the maximum amount of extractable melt to 0.35 at each node requires complete melt extraction at three nodes of layer 3 before appearance of a new node in layer 2. For simplicity, we neglect both the effects of latent heat of crystallization and convection within the growing magmatic bodies, imposing to new nodes a starting temperature close to that of relevant minimum melts. Although this model of thermal exchange certainly represents an oversimplification of partially molten systems, the errors are expected to be minimal due to the 1D nature of the code. The amount of melt extracted at every node for the current time step ($M_f^t$) is calculated taking into account the cumulative volume of already-extracted melt, as:

$$M_f^t = M_0 - \sum_{i=1}^{t-1} M_i^t$$

where $\sum_{i=1}^{t-1} M_i^t$ is the total volume of melt extracted during the previous time steps, and $M_0$ is a standard amount of extractable melt (Vogt et al., 2011). Therefore, layer 2 becomes refractory as temperature remains above the solidus of tonalite and eventually stops melting when $\sum_{i=1}^{t-1} M_i^t > M_0$.

### 2.5 Deformation and rheology

Provided that deformation involves simple shear, in one dimension the heat production rate due to shearing ($H_s$) is calculated from the equation (Turcotte and Schubert, 2002; Burg and Gerya, 2005):

$$H_s = \sigma \cdot \dot{\varepsilon}$$

where $\sigma$ is deviatoric stress (Pa) and $\dot{\varepsilon}$ denotes the strain rate (s$^{-1}$). Eq. (9) indicates that shear heating is proportional to stress, therefore it is expected to decrease as temperature increases because of stress dependence on $T$ (Fig. 2). In our experiments, strain rate is assumed to be constant within the deforming zone (Platt & Behr, 2011), whereas stress in solid rocks ($M_j < 0.1$) is calculated as a function of temperature using a power-law flow law of the general form:
where $A_j$ is a pre-exponential constant (MPa$^{-n}$ s$^{-1}$), $Q_j$ is activation enthalpy (kJ mol$^{-1}$), $R$ is the gas constant, and $n_j$ is the stress exponent. The effect of shear heating is evaluated at nodes of layer 2 and 3 by substituting into Eq.(9) the stress values calculated from Eq.(10) using flow law parameters of wet quartzite (Gleason and Tullis, 1995). Olivine parameters (Hirth and Kohlstedt, 2003) are used to simulate the rheology of sub-continental mantle (Table 1). Because of inverse temperature dependence of stress (eq. 10), for realistic strain-rates on the order of $10^{-12} – 10^{-15}$ s$^{-1}$ shear heating become generally negligible ($< 0.01 \mu$W m$^{-3}$) some 2 to 3 nodes below the brittle-ductile transition, therefore shear heating is effectively treated as a self-regulating mechanism. The rheology of partially molten rocks ($M_j> 0.1$) is calculated as $\eta_j = \frac{\eta_0 e^x}{1 + (M_j)^x}$, where $\eta_j$ is the effective viscosity calculated according to the following equation (Pinkerton and Stevenson, 1992; Bittner and Schmeling, 1995):

$$\eta_j = \eta_0 \exp \left[ \frac{2.5 \times (1 - M_j) e^{\left(\frac{2.5 - M_j}{M_j}\right) 3.87}}{1 + (M_j)^x} \right]$$

where $\eta_0$ is an empirical parameter that ranges from $10^{13}$ Pa s in molten mafic rocks to $5 \times 10^{14}$ Pa s in felsic rocks. For simplicity, the crust is assumed to be overall felsic. In all numerical simulations, effective viscosities of between $6 \times 10^{15}$ and $8 \times 10^{16}$ Pa s are obtained for the partially molten crust indicating a significant stress drop of 3 to 6 orders of magnitude.

### 3. Numerical modeling

The software is tested on the HT metamorphic event recorded across the South Variscan Belt during the Carboniferous–Permian transition. The source of such a regional-scale HT gradient is a topic that remains controversial. Such an event may have resulted from selective enrichment in heat-producing elements due to crustal reworking (Lexa et al., 2011), focused shear heating (Nabelek and Liu, 1999; Burg and Gerya, 2005), or from upwelling of hot asthenosphere due to slab break-off (Cocherie et al., 1994; Ledru et al., 2001; Vilà et al., 2007; Gébelin et al., 2009; Faure et al., 2010). The numerical solutions of Eq.(6), computed using GEOTHERM, are used here to test the applicability of either of these end-member models starting from a geologically reasonable configuration of the modeled crust in terms of its thickness and composition.
3.1 South Variscan Belt

The South Variscan Belt (SVB) formed during Late Devonian to Carboniferous times, between approximately 360 and 300 Ma (Lardeaux et al., 2001; Paquette et al., 2003; Giacomini et al., 2005; Giacomini et al., 2006; Bellot and Roig, 2007; Faure et al., 2010). Most authors distinguish a phase of major crustal thickening from early Devonian to around 350 Ma, followed by general extension until the Carboniferous–Permian transition. Most of the shortening phase was coeval with Barrovian metamorphism, exhumation of high-pressure (HP) granulitic domes, and partial melting of the felsic crust at amphibolite facies conditions (350–340 Ma, Giacomini et al., 2006; Cruciani et al., 2008; Casini et al., 2009; Faure et al., 2010). Extension and thinning of the previously thickened crust is generally associated to the emplacement of large volumes of anatectic melts (Rossi and Cocherie, 1991; Rossi et al., 2009; Casini et al., 2012) and the development of a widespread HT-LP metamorphic province characterized by andalusite/sillimanite ± cordierite assemblages and low-pressure anatexis (Giacomini et al., 2006; Rossi et al., 2009; Casini et al., 2012). The beginning of extension was probably diachronous along the SVB, as indicated by considerable variation in the exhumation ages and cooling path trajectories of lower crustal units. Although inferred exhumation rates range from 3–1.5 mm y\(^{-1}\) to 0.3–0.1 mm y\(^{-1}\) depending on the structural level (Henk, 1995; Lardeaux et al., 2001; Casini et al., 2010; Fornelli et al., 2011), it is generally accepted that the European Variscan crust reached a stable thickness similar to the present configuration (Moho at 35–40 km depth) in the early Permian (Grad et al., 2009).

Based on structural analysis, paleogeographic reconstructions, and geochronology, the transition from shortening to extension and the late Carboniferous – early Permian HT metamorphic event is characterized by the development of lithospheric shear zones (Carosi and Oggiano, 2002; Dallagiovanna et al., 2009; Gebelin et al., 2009; Martinez Catalan, 2011; Casini et al., 2012; Maino et al., 2012). One of these structures, running from the Bohemian Massif to Morocco along the axis of the SVB, is supposed to have accommodated some 50–300 km of horizontal displacement from about 320 to 290 Ma, involving ductile deformation of the lithosphere with average strain rates from \(10^{-13}\) to \(10^{-14}\) s\(^{-1}\) (Tartése et al., 2011; Martinez Catalan, 2011).

3.2 Model set-up

Values for the compositional parameters of the crustal model, such as the \(^{235,238}U\), \(^{232}Th\), and \(^{40}K\) contents (Table 2), and model densities, were selected on the basis of published data sets (Lucazeau and Mailhe, 1986; Cocherie et al., 1994; Verdoya et al., 1998; Labani et al., 2006; Puccini et al., 2013). Deep seismic profiles through Variscan Europe show an average Moho depth of about 35–40
km, the higher values being preserved in regions unaffected by post-Variscan extension (e.g., Guy et al., 2011; Grad et al., 2009). Based on the observed levels of exhumation of metamorphic units and emplacement depths of early Permian plutons (Vilà et al., 2007; Gébelin et al., 2009; Faure et al., 2010; Tartèse et al., 2011; Casini et al., 2012), a reference bulk crustal thickness of 70 km is assumed at the beginning of the experiments (350 Ma). The Moho is generally thought to have reached a stable depth in the early Permian, so a bulk crustal thickness of 40 km is imposed at the end of experiments. The crust is internally subdivided into three layers: i) layer 1 (L1), upper crust composed of sedimentary rocks and synorogenic sediments; ii) layer 2 (L2), middle crust of mainly felsic metamorphic rocks and granites; and iii) layer 3 (L3), lower crust of felsic and mafic granulites in variable proportions (O’Brien and Rötzler, 2003). The estimate for the thickness of layer 1 is based on the thickness of Carboniferous synorogenic basins preserved in this region of the chain (Echtler and Malavieille, 1990). Because of post-Variscan exhumation, the observed 2-4 km-thick Carboniferous sedimentary sequences would represent a minimum estimate for the upper crust, which is thus assumed to be L1 = 7 km, a value close to the actual thickness of synorogenic basins in the Himalaya. The lower crust is constrained using present-day seismic profiles and petrologic arguments. Seismic tomography data for the Corsica–Sardinia block (Finetti, 2005) and for central Europe (Guy et al., 2011) suggest a present-day 17–22-km-thick granulitic lower crust. Provided that late Carboniferous and early Permian granitic/tonalitic batholiths (average thickness 6 – 10 km) were sourced in the lower crust (Rossi and Cocherie, 1991; Ferré and Leake, 2001; Cruciani et al., 2008), the initial thickness of the granulitic layer is calculated as L3 = 28 km to balance the volume of removed material. The initial thickness of the middle crust (L2 = 35 km) is calculated by difference, using a reference bulk initial thickness of 70 km (Table 2).

The first set of numerical experiments (R1–R3, Table 3) simulates the effect of variable exhumation rates. Exhumation rates are assumed to change within a range of values extrapolated from published geologic constraints (Henk, 1995; Lardeaux et al., 2001; Casini et al., 2010; Fornelli et al., 2011). The first experiment (R1) uses high exhumation rates (2 mm y⁻¹) in the first 10 Myr and much lower rates (0.25 mm y⁻¹) in the following 40 Myr. Experiment R2 assumes low exhumation rates (0.33 mm y⁻¹ in the first 30 Myr) followed by higher exhumation rates of 1 mm y⁻¹ from 320 to 300 Ma. Finally, experiment R3 uses extremely high exhumation rates of 2.5 mm y⁻¹ in the first 10 Myr and then extremely low rates (0.12 mm y⁻¹) until the end. In all of these experiments, shear heating is assumed to be insignificant and is set to zero. The slab break-off model is explored in experiments R4–R8 (Table 3), by imposing the rise of hot asthenosphere beneath the Moho at progressively younger ages, from 345 up to 310 Ma, close to the age of HT metamorphism. The effect of shear heating is evaluated in a third set of experiments (R9 to R12), using variable strain...
rates and durations of the event (Table 3). The last numerical experiment (R13, Table 3) is performed based on the boundary conditions (i.e., age of break-off, age and intensity of shearing, and exhumation rates) that best fit thermobarometric constraints. This simulation therefore prescribes relatively low exhumation rates (0.78 mm y\(^{-1}\)) in the first 28 Myr and then even lower (0.36 mm y\(^{-1}\)) until the end. Slab break-off is imposed at 342 Ma, whereas shearing occurs between 318 and 305 Ma at an average strain rate of 10\(^{-13}\) s\(^{-1}\).

4. Results

The results of numerical experiments were compared with independent thermobarometric constraints (Table 4) obtained from several units distributed along the root zone of the South Variscan Belt (Fig. 3). The solidus/liquidus curves of wet granite (Johannes and Holtz, 1996) and the aluminosilicate stability fields (Richardson et al., 1969) are also displayed for reference. In all experiments (Figs 3-6), the surface heat flow ranges between 125 and 105 mWm\(^{-2}\), a value range consistent with present-day estimates in regions of thickened crust such as the Himalaya (Sclater et al., 1980; Jaupart and Mareschal, 2007). The Moho heat flow is more variable, depending on the imposed tectonic model; peak values between 30 and 35 mWm\(^{-2}\) (Figs 3,5) are obtained in experiments 4–8 and 13 at a few Myr (generally <10) after slab break-off, consistent with the inferred timescale for thermal relaxation (Davies and von Blanckenburg, 1995). The fit of the model to petrologic data is evaluated at every time step using the available constraints within their appropriate time spans (Figs 3-6). The relative error is calculated as the median difference (%) between the numerical geotherm and the second-order polynomial fit to P–T–t points, within the region of the profile where thermobarometric constraints are available. Therefore, negative errors indicate that numerical models overestimate the actual temperatures inferred from thermobarometry, whereas positive values reflect underestimation.

4.1 Variable exhumation rates

The first three experiments (Fig. 4) simulate a thermal evolution controlled only by exhumation and erosion. Partial melting of the lower crust occurs early in experiments 2 and 3, from 350 to about 340 Ma. However, the volumes of mobilized melts are small, between 0.04% and 0.12%, involving a limited thinning of the lower crust whose thickness remains in the range 26.5–24 km at 300 Ma; therefore, in models controlled by exhumation and erosion, only 2–4 km of lower crustal material is transferred to the middle crust and made available for the assembly of granitic batholiths. The relative error between the petrologic constraints and calculated geotherms is smallest in experiment 2 (Fig. 4), and is substantially higher in experiments 1 and 3, where initially high exhumation rates
decrease during the last 40 Myr of the experiments. However, all experiments show a considerable mismatch and do not reproduce the typical HT metamorphic conditions in the andalusite–biotite–cordierite stability fields recorded by the Variscan crust between 310 and 300 Ma (Giacomini et al., 2006; Vilà et al., 2007; Casini and Oggiano, 2008; Cruciani et al., 2008; Faure et al., 2010). Specifically, errors of up to about +30% indicate that the calculated geotherms significantly underestimate the actual temperature distribution in the upper 15 km of the crust.

4.2 Slab break-off at variable times

In experiments 4–8 (Fig. 5), exhumation rates are 0.6 mm y\(^{-1}\) in the first 30 Myr, and decrease slightly to 0.5 mm y\(^{-1}\) from 320 to 300 Ma (Table 3). Slab break-off is simulated by imposing a sudden change in temperature within a 12-km-thick layer that approximates the rise of hot, low-viscosity asthenospheric material (\(T = 1630\) K) beneath the Moho. The consequences for the crustal geotherm are evaluated 5 Myrs after slab breakoff, at different ages from 345 to 305 Ma (Fig. 5a-e); that is, slab breakoff is imposed at ages progressively closer to the age of HT metamorphism. A common feature of these experiments is efficient melting of the lower crust, which causes the final thickness of the granulitic layer to be 18.2–19 km. Although the 1D nature of the code does not allow a reproduction of the effective melt pathways and possible loss of melt on the way to the emplacement regions, the large amount of melt potentially extracted is consistent with the development of 6–8-km-thick granitic plutons and batholiths. The relative error between the petrologic constraints and calculated geotherms is strikingly similar in all experiments (Fig. 5f), and remains below a value of +15% during the HT event (310–300 Ma, Fig. 5). The calculated temperature distribution underestimates the actual temperature distribution recorded by mineral assemblages in the shallower part of the crust.

4.3 Variable age and magnitude of shear heating

Experiments 9–12 evaluate the effect of shear heating in the absence of slab break-off (Fig. 6), using the same exhumation rates as those of experiments 4–8 (Table 3). Shearing is imposed at 320 Ma and variable strain rates from \(10^{-16}\) to \(10^{-13}\) s\(^{-1}\) are assumed, consistent with geological constraints. In all experiments, melting of the lower crust is observed from 350 to about 335 Ma. Nevertheless, the melting rates and the bulk volume of extracted melt are slightly lower than those predicted by experiments 4–8; therefore, the lower crust presents a final thickness of between 20 and 22 km depending on the magnitude of the shear strain rate. The relative error of numerical geotherms is similar in experiments 9–11 (Fig. 6), and still reflects an underestimation of the effective temperature at shallow crustal levels at around 310–300 Ma. The best fit (−6%) to the HT
event is provided by experiment 12, which assumes an average strain rate of $10^{-13}$ s$^{-1}$, close to the upper bound of geologically realistic values for lithospheric structures (Brace and Kohlstedt, 1980).

4.4 Composite extensional model

The last numerical experiment is used to demonstrate the combined effects of shearing and slab break-off (Fig. 7). Based on general exhumation models for the SVB, exhumation rates are assumed to decrease discontinuously from an initial value of 0.78 to 0.36 mm y$^{-1}$ at the Carboniferous–Permian transition (Table 3). The rise of hot asthenospheric mantle is imposed at 342 Ma, that is 5 to 7 Myr before emplacement of Mg–K granites (Rossi and Cochere, 1991; Paquette et al., 2003). These rocks were derived primarily from the mixing of anatectic and mantle-derived melts extracted at the crust–mantle interface and therefore represent a likely record of the thermal pulse related to slab break-off (Rossi and Cochere, 1991; Ferré and Leake, 2001; Paquette et al., 2003). A shear event with an average strain rate of $10^{-13}$ s$^{-1}$ is applied at the end of Carboniferous between 318 and 305 Ma; the age of deformation is extrapolated from published geochronological constraints for major shear zones and shear-related syntectonic granites (Gébelin et al., 2009; Tartése et al., 2011; Casini et al., 2012). As shown in Figure 6, partial melting of the lower crust yields a final thickness of 18.2 km. Although melting is potentially a continuous process, the volume of extracted melt rises suddenly a few million years after breakoff of the slab. This causes the lower crust to become essentially refractory at around 338 Ma. The relative error of the geotherm and petrologic constraints is consistently within ±10% and decreases to about +2% during the 310–300 Ma period, providing the best fit to the HT event.

5 Discussion and conclusions

GEOTHERM has been tested by simulation of the transient geotherm developed across the South Variscan Belt from the early Carboniferous to the Carboniferous–Permian transition. Results of 1D thermal models indicate that P–T–t constraints around 310 and 300 Ma cannot be fitted by near-contemporaneous slab break-off, which would have generated unrealistically high temperatures close to the Moho but without providing the required heat at shallower depth (Fig.4). This observation is in good agreement with the inferred timescale of heat propagation after break-off in the order of 10–15 Myr (Davies and von Blanckenburg, 1995). Experiment 13 provides a good fit to petrologic data (Fig. 7), and produces a final configuration of the crust in close accordance with geophysical observations that indicate 18 km of granulitic lower crust (O’Brien and Rötzler, 2003; Guy et al., 2011). In experiment 13, the break-off is imposed at 342 Ma; that is, a few Myr before
emplacement of the Mg–K granites (e.g., Paquette et al., 2003). Placing the slab break-off in the early Carboniferous provides geologically reasonable geotherms that fit the age of Barrovian-type and HP mineral assemblages, particularly if a component of shearing of $10^{-13} \text{s}^{-1}$ is introduced at 322 Ma (Fig. 7). This configuration provides the best fit (error $< \pm 5\%$) to the Carboniferous–early Permian HT event recorded by metamorphic mineral assemblages. The results of experiment 13 suggest that late Variscan HT metamorphism was not a consequence of a near-coeval increase of heat flow across the Moho; that is, the thermal effects of slab break-off do not by themselves explain the development of the high temperature gradient at shallow crustal levels, which is instead best explained in terms of crustal attenuation and the selective enrichment of heat-producing elements coupled to intense, though realistic, shear heating.

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**Figure captions**

**Figure 1.** Numerical grid: $T$ is temperature [K], $dz$ is spatial derivative [m], $dt$ is temporal derivative [s], $\kappa$ is thermal diffusivity [ms$^{-1}$], the superscripts $n$ and $n+1$ denote the current and future time step, respectively. The subscript $l$ and $nz$ indicate the upper and lower boundary points of the grid, respectively, and the subscript $j$ denotes position of intermediate nodes.

**Figure 2.** $T$ vs $H_s$ plot: the curves show the relation between shear heating and temperature for constant strain rates between $10^{-12}$ and $10^{-16}$ s$^{-1}$.

**Figure 3.** Schematic structural sketch map of the European Variscides; the place of the South Variscan Belt (SVB) is indicated. Black dots represents thermobarometric constraints in the range 350 – 325 Ma, white dots stand for constraints < 325 Ma (see Table 3 for references); samples are indicated with the same lettering as in Table 4. BM: Bohemian Massif; MGCR: Mid German Crystalline Rise; ECM: External Crystalline Massifs of the Alps; MC: French Massif Central; CIZ: Central Iberian Zone; C-S: Corsica-Sardinia Massif; PAL: Posada-Asinara Line (Rossi et al., 2009).
Figure 4. Variable exhumation rate experiments. The main plot (left) displays the temperature[K]/depth[km] distribution profiles obtained assuming variable exhumation rates; the sharp increase of T at around 15 km depth and 345 Ma is due to upward migration of lower crustal melts (see table 3 for details of experimental inputs). The upper-right plot shows the relative error [%]/age [Ma] plot obtained from step-by-step comparison of petrologic constraints and the numerical geotherms. The lower-right plot shows the calculated heat flows [mW m⁻²] at progressively younger ages (solid lines = surface heat flow, dotted line = Moho heat flow). In Figure 3 and followings, the gray solid lines showed in the main plot indicates the stability field of aluminosilicates (Richardson et al., 1969); the gray dotted lines represent the hydrated granite solidus and liquidus curves (Johannes and Holtz, 1996).

Figure 5. Variable break off age experiments: a-e) plots displaying the temperature[K]/depth[km] distribution profiles obtained 5 Myrs after slab breakoff for progressively younger ages of slab break off (see table 3 for details of experimental inputs); both the geotherm and the model geometry at 300 Ma (age of HT metamorphism) are also displayed for comparison; f) the upper-right plot shows the relative error [%]/age [Ma] plot obtained from step-by-step comparison of petrologic constraints and the numerical geotherms. The lower-right plot shows the calculated heat flows [mW m⁻²] at progressively younger ages (solid lines = surface heat flow, dotted line = Moho heat flow).

Figure 6. Variable shear intensity experiments. The main plot (left) displays the temperature[K]/depth[km] distribution profiles obtained assuming decreasing intensity of shear, from 10⁻¹⁶ to 10⁻¹³ at 320 Ma (see table 3 for details of experimental inputs). The upper-right plot shows the relative error [%]/age [Ma] plot obtained from step-by-step comparison of petrologic constraints and the numerical geotherms. The lower-right plot shows the calculated heat flows [mW m⁻²] at progressively younger ages (solid lines = surface heat flow, dotted line = Moho heat flow).

Figure 7. Composite extensional model experiment. The main plot (left) displays the temperature[K]/depth[km] distribution profiles obtained from 345 to 300 Ma (age of relevant curves displayed) assuming that age of break off is 342 Ma. A 10⁻¹³ shear event is imposed from 318 to 307 Ma. The upper-right plot shows the relative error [%]/age [Ma] plot obtained from step-by-step comparison of petrologic constraints and the numerical geotherms. The lower-right plot shows the calculated heat flows [mW m⁻²] at progressively younger ages (solid lines = surface heat flow, dotted line = Moho heat flow). The initial configuration of the model crust is shown in the left side of the main plot (see Table 2 for layer composition and thickness).
Table 1.

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Table 2.

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Table 3.

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Table 4.
Transient Variscan geotherms are calculated using a Matlab-derived package. The heat equation is solved in 1D using temperature dependent thermal conductivity. The software has been tested on the evolution of the Corsica-Sardinia Batholith. The geotherms match petrologic constraints for early Carboniferous break off. Results argue against direct linkage between slab break off and HT metamorphism.
Figure 1
Temperature [K]

Hs [$\mu$Wm$^{-3}$]

Figure 2
Figure 3

Variscan Europe
- External thrust belt and foredeep basin (Avalonian terranes)
- Gondwanan terranes with strong Cadomian imprint
- Gondwana fold and thrust belt
- Variscan strike slip faults
- Alpine front
- South Variscan Belt (SVB)

PT constraints (360 - 325 Ma)
PT constraints (325 - 300 Ma)

Suprastructure (Moldanubian-type terranes)
Variscan strike slip faults
Variscan front and foredeep basin (Avalonian terranes)
Gondwanan terranes with strong Cadomian imprint
Gondwana fold and thrust belt
Figure 6
Figure 7

- Temperature (K) vs. depth (km)
- Best fit/age
- Error [%] vs. age (Ma)
- Heat flow (mW/m²) vs. age (Ma)
- Experiments:
  - exp.13
  - 350-325 Ma
  - 325-300 Ma
- Depth:
  - Initial Moho
  - Moho (300)
  - Lower crust
  - Middle crust
  - Upper crust
- Temperature:
  - Overestimated
  - Underestimated
- Shaded areas indicate:
  - Temperature overestimated
  - Temperature underestimated

Graphs and diagrams illustrate the relationship between temperature, depth, error, and age across different crustal layers and experimental conditions.