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Natural equivalents of thermal gradient experiments

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ABSTRACT

Crystallization experiments using the intrinsic thermal gradient in 10 mm length capsules loaded in piston-cylinder assemblies were used to investigate silicic magma crystallization. The application of experimental results to natural environments requires the scaling of physical parameters of petrological interest. Therefore, we propose here a comparative study between thermal gradients and numerical simulations of natural magma chambers. We use the Finite Element Method to calculate thermal profiles across a cooling silicic magma chamber. These numerical profiles are compared with the intrinsic thermal structure of half-inch, piston-cylinder assemblies at 500 MPa. It is concluded that a set of varied magma chamber geometries and/or distinct stages of their cooling history can approach the intrinsic thermal structure of laboratory experiments. Once the thermal properties for magma and its host rock are fixed, the experimental-numerical approach is mostly dependent on the volume and aspect ratio of the magma chamber. Our results indicate, for instance, that a 10 mm length capsule with a thermal gradient of 40 °C/mm (from 1100 to 700 °C) may represent a 150-1100 m wide portion of a cooling magma chamber of 10-20 km diameter and 2-10 km height, emplaced at a depth of 18 km. Additional possible scenarios are represented by larger magma

chambers, up to 30 km diameter, in which the experimental thermal gradient can represent a 150-3700 m-thin-section of the large igneous bodies.

1. Introduction

Experimental petrology apparatus, like the piston-cylinder (Boyd and England, 1960), were designed to simulate natural conditions in small capsules in which temperature (and pressure) is constant over their entire volume; a requirement to reproduce phase compositions in laboratory through the control of intensive variables. However, outside a restricted area (*hotspot*) of about 5 mm diameter, strong thermal (intrinsic) gradients develop in piston-cylinder assemblies (Lundstrom et al., 2005; Huang et al. 2009; Watson et al., 2002). The thermal gradient is controlled by a number of factors such as capsule length, assembly design, pressure transmitting solid media, and the pressure and temperature used (Schilling and Wunder, 2004).

Thermal gradient measurements in piston-cylinder are firstly affected by the large conductivity of the metal capsule that buffers the thermal difference across the assembly. Thus, the thermal structure of a piston-cylinder will also depend on the length, diameter and the metal composition of the capsule. The use of different materials in the solid pressure transmitting media can affect thermal gradient depending on its thermal conductivity. Moreover, temperature and pressure conditions can affect the thermal conductivity of solid pressure media. Previous experimental works (Pickering et al., 1998; Watson et al., 2002) and numerical modelling (Schilling and Wunder, 2004) were performed to constrain thermal profiles in experimental assemblies with marked differences with respect to our design. Hence, new experiments are

required to better constrain the thermal gradient in half-inch assemblies loaded with the longer capsules.

The point of interest is that in using long capsules (>5 mm length), it is possible to take advantage of the intrinsic thermal gradient in order to simulate the crystallization of shallow magma chambers, which cool from their walls to the innermost part (Huang *et al.*, 2009, Masotta *et al.*, 2012, Mollo and Masotta, 2014). Preliminary results are of great value to gain intuition on processes in magma chambers; however the transfer of experimental results to km-sized magma bodies is not a straightforward process. Here we present the scale of application to km-sized magma bodies in nature. With this purpose, we have compared intrinsic thermal gradients in piston-cylinder experiments and magma chamber gradients inferred by means of thermomechanic numerical modelling.

Experimental thermal profiles are compared with those resulting from numerical simulations reproducing natural magma chambers at different stages of their cooling history. In both capsules and selected magma chambers, the whole temperature range that encompasses *liquidus* to *solidus* conditions (Fig. 1) of intermediate andesitic systems ($\text{SiO}_2 \approx 60$ wt%) has been reproduced. The relevant issue for the scaling is to infer what the conditions are in terms of magma chamber geometry, size and evolutionary stage, for which the experimental-natural comparison is relevant. The geometry of the gradient curve from *liquidus* to *solidus* depends on magma chamber parameters such as the diameter, depth of emplacement and cooling time period. Our results indicate that intrinsic experimental gradients can fit only a limited set of natural conditions. Hence, caution must be exercised for the application of thermal gradient experiments to settings outside those recommended here.

2. Rationale

It is known from experiments and thermal modelling of piston-cylinder assemblies (Huang et al., 2009; Masotta et al., 2012; Pickering et al., 1998; Schilling and Wunder, 2004; Watson et al., 2002) that large thermal gradients occur inside the graphite furnace. Temperature is constant over a short distance of about 5 mm from the centre of the furnace and drops suddenly to much lower values towards the bottom and the top. Interestingly, the *liquidus-solidus* interval can be covered by this intrinsic thermal gradient, opening new possibilities to study magma differentiation processes.

The scaling of this intrinsic experimental thermal gradient may be performed by direct comparison of the thermal structure within the graphite furnace with that of a km-sized magma chamber. By contrast, the kinetic processes responsible for the experimental results cannot be scaled only through the thermal properties of piston-cylinder apparatus. The results from laboratory experiments shed light to specific phenomena constrained to limited portions of a magma chamber. The aim of this work is to delimit the equivalence of this portion in nature by means of the thermal structure imposed in these experiments. To do so, we present a new approach to scale thermal gradient experiments to natural systems. On the one hand, the intrinsic thermal gradient is directly measured by using special assemblies equipped with double thermocouples. On the other hand, natural gradients of km-sized magma chambers are calculated by means of numerical modelling. The latter consists of a time-dependent thermal model that simulates the cooling process of a closed magmatic system embedded in a colder and homogeneous host rock. To achieve this comparison, we extrapolate the entire capsule length to natural cases (Fig. 1).

We use as an example of application the experimental thermal profile in which the hotspot is constrained to the *liquidus* of a given standard andesitic composition. In any case, this process can be repeated for different magma compositions or experimental thermal set-ups. It must be noted that it is not possible to explore all possible combinations of the mentioned parameters in the current paper and that it may be addressed in future works.

The intrinsic thermal gradient is directly measured by using special assemblies equipped with double thermocouples. The natural gradients of km-sized magma chambers are calculated by means of numerical modelling. Shedding some light on the natural equivalence of the experimental thermal gradient allows a better understanding of the experimental results as pertaining to magma chambers of different sizes and evolutionary stages, and/or to different portions of magma chambers. It is worth noting that the thermal gradient can be correlated either to the initial cooling representative of a small fraction (Fig. 1a) of the chamber near the wall rocks, or to more advanced stages of cooling associated to higher degrees of crystallization (Fig. 1b). The results obtained here indicate that the thermal gradient, imposed over the entire capsule length, allows us to simulate various evolutionary stages of the same magma chamber and/or different magma chambers within a wide range of sizes and geometries.

3. Calibration experiments of thermal gradients in piston-cylinder apparatus

3.1. Experimental techniques

The experiments were designed to calibrate the thermal gradient operating in the capsule. Runs were carried out using a double thermocouple set up in order to measure the temperature gradient. The thermocouples measured temperatures from 900 to 1200

°C over a constant pressure of 500 MPa. Calibration experiments were performed in a Boyd-England type piston-cylinder apparatus installed at the University of Huelva (Spain). The two thermocouples are positioned in a "special periclase assembly". This assembly is made up of a 12.5 mm (half inch) diameter, talc-pyrex-periclase cell, Au-Pd capsule and drilled periclase. Gold-Palladium ($\text{Au}_{70}\text{Pd}_{30}$) capsules of 3 mm diameter, 10 mm length, and 0.15 mm wall were filled with drilled periclase that serves (1) to simulate the sample effects on the gradient and (2) to ensure that the thermocouple is at the desired position with respect to the centre of the furnace (Fig. 2). Then, the capsules were introduced into MgO pressure containers.

The temperature was measured and controlled with two $\text{Pt}_{100}\text{-Pt}_{87}\text{Rh}_{13}$ thermocouples connected to Eurotherm 808 controllers, with estimated uncertainties of ± 1 °C. The first thermocouple is positioned at the centre (hotspot) of the furnace (hereinafter called *control position*; CP in Fig. 2). The second thermocouple (hereinafter called *measure position*) is located at two different distances from the centre of the furnace (6.6 and 10 mm corresponding to MP1 and MP2 in Fig. 2). In this way, the temperature at these measure positions was calibrated by two different experiments (CG1 and CG2). A dwell time of 20 minutes was needed to reach thermal equilibrium within the assembly in order to make temperature oscillations negligible. Temperature and power supply data were recorded automatically within 1-min time intervals.

The oil pressure was measured with electronic DRUCK PTX 1400 pressure transmitters, connected to OMRON E5CK controllers. The value of pressure was manually corrected and maintained within a narrow range of ± 5 bar oil pressure, equivalent to ± 250 bar on the sample. Pressure was maintained at 500 MPa in all the experimental runs. The initial temperature was fixed at 1200 °C for two hours to ensure the stability of the thermocouple measurement and then, different cooling ramps were

applied to test the response of the thermal gradient to cooling. The final temperature was set at 1130 °C and 800 °C for the CG1 and CG2 runs, respectively. A complete list of experimental conditions is given in Table 1.

The small deformation and compaction of our well-packed assemblies did not modify significantly the initial distance of the control thermocouple to the centre of the furnace (hotspot). After extraction of the assembly, we checked the following points for each run: (1) the control thermocouple is placed within the hotspot (Fig. 2, CP); (2) the measure thermocouple is in the desired position along the thermal gradient (MP1 and MP2 in Fig. 2); (3) the distance between both thermocouples, control and measure, is coincident with that of the initial setup (Fig. 2); (4) the distance between the bottom of the furnace and the measure thermocouple coincides with that of the initial setup (MP1 and MP2 in Fig. 2).

3.2. Calibration experiment results

Thermal gradient calibrations define the whole thermal distribution along the piston-cylinder assembly. The output temperature values were acquired with a continuous data acquisition system wired to both thermocouples. The systematic variation according to the programmed temperature decrease, at both thermocouple measure positions (Fig. 3) shows a stable thermal structure for the experimental assembly.

The temperature at the hotspot is established according to the *liquidus* temperature of the selected magma composition for the numerical modelling. The thermal gradient experiment with the hotspot set at 1106 °C (i.e. the *liquidus temperature of AGV-2, see Physical and thermal properties of the magma and its country rock* for further explanations on the selected composition) is compared with the numerical models. The temperatures measured at 6.6 and 10 mm from the 1106 °C hotspot are calculated using

the linear regression equation showed in Fig. 3a and b, respectively. The derived values define the experimental thermal gradient that is later compared with the numerical thermal profiles (Table 2).

4. Numerical simulation of natural magma chambers

4.1. Theory and equations

Mathematical modelling techniques have proved by far their applicability to the study of processes driving magma chamber evolution (Annen, 2009; Bachmann, 2004; Bachmann, 2006; Bea, 2010; Gelman et al., 2013; Gutiérrez and Parada, 2010; Huber et al., 2009; Huber et al., 2012; Koyaguchi, 2001). Here, the internal temperature distribution of the magma chamber is calculated using the Finite Element (FE) method, by solving the heat transfer equation, assuming as negligible the effect of viscous heating and pressure-volume work:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \nabla T = \nabla(k \nabla T) + \mathbf{Q} \quad (1)$$

where the equation parameters refer to density (ρ), specific heat capacity at constant pressure (C_p), temperature (T), time (t), the velocity vector ($\mathbf{u}$), thermal conductivity (k) and $\mathbf{Q}$ contains heat sources other than viscous heating (see Table 3 for more details concerning thermal and physical parameters). Since we are dealing here with pure conductive heat transfer (i.e. $\mathbf{u}=0$), Equation (1) can be rearranged as follows:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla(-k \nabla T) = \mathbf{Q} \quad (2)$$

As in previous published works (e.g. Gelman et al. 2013), the present models do not consider heat transfer by convection within the magma chamber. It has been reported that slow convection cells are limited to the liquid core of a cooling pluton (Bea, 2010), not affecting the partially crystallized zone of the solidification front where we apply

our study. In the case of cooling silicic magma chambers, the convective effect has been attributed to initial short melting stages after basalt replenishment during which the temperature at the solid-liquid boundary exceeds the effective fusion temperature (Koyaguchi & Kaneko 2000). Basalt replenishment has not been taken into account for the objectives of this study. On the basis of the above considerations and for the sake of simplicity, convection has been omitted in the equations and the results here presented only apply to this set of conditions. Boundary layer processes as thermal or compositional changes that can influence the cooling of magma chambers (Lundstrom et al. 2005) are considered as negligible for the purpose of the comparison between experimental and natural processes.

The geometric modelling, mesh discretization and numerical computations were carried out with COMSOL Multiphysics v4.4 software package (<http://www.comsol.com>). To simulate the solidifying magma, we use the *heat transfer with phase change* module. The latter allows solving the heat equation after setting the properties of a phase-change material (from liquid to solid) according to the Apparent Heat Capacity formulation (AHC) (Canot et al., 2009; Hu and Argyropoulos, 1996; Voller et al., 1990). By convention, COMSOL Multiphysics v4.4 considers magma to be in phase 1 when it is completely solid and in phase 2, when fully liquid. The phase-change interval (ΔT) is then defined as the temperature range where phase 1 and 2 co-exist. In our case, it covers then from the *liquidus* ($T_{liquidus}$) to *solidus* ($T_{solidus}$) temperatures, i.e. $\Delta T = T_{liquidus} - T_{solidus}$ (Fig. 4a).

The AHC method is the best for naturally occurring wide phase-change temperature interval, as is the case of magma cooling where ΔT may be up to 500°C. The latent heat of crystallization is accounted for by increasing the heat capacity of the material within the temperature range of the phase change (Canot et al., 2009; Hu and Argyropoulos,

1996; Voller et al., 1990). Thus, rather than to introduce the latent heat L into the energy balance equation, when the material reaches its phase change temperature T_{pc} , it is assumed that the transformation occurs in a temperature interval between $T_{pc}-\Delta T/2$ and $T_{pc}+\Delta T/2$ (Fig. 4a). In this interval, the solidifying magmatic system is modelled as a function of ς and α , where $\alpha = 1 - \varsigma$, representing the fraction of phase 1 and 2 (i.e. solid and liquid) during the phase change interval, respectively. According to the formulation, α is equal to 0 before $T_{pc}-\Delta T/2$ and to 1 after $T_{pc}+\Delta T/2$. In the present models:

$$T_{pc} - \frac{\Delta T}{2} = T_{solidus} \quad (3)$$

$$T_{pc} = \frac{T_{liquidus} - T_{solidus}}{2} \quad (4)$$

$$T_{pc} + \frac{\Delta T}{2} = T_{liquidus} \quad (5)$$

The enthalpy H of the system is:

$$H = \varsigma H_{solid} + \alpha H_{melt} \quad (6)$$

where H_{solid} and H_{melt} are the enthalpies when the material is solid or liquid, respectively. Differentiating with respect to temperature, we obtain the following expression for the specific heat capacity at constant pressure:

$$Cp = \varsigma Cp_{solid} + \alpha Cp_{melt} + (H_{solid} - H_{melt}) \frac{d\alpha}{dT} \quad (7)$$

which can be rewritten as:

$$Cp = \phi Cp_{solid} + \theta Cp_{melt} + (H_{solid} - H_{melt}) \frac{d\theta}{dT} \quad (8)$$

where we have substituted the smoothing functions α and ς imposed by default in COMSOL with the temperature dependent melt (θ) and solid (ϕ) fractions of the crystallizing magma (Table S1, Supplementary material).

Thus, according to Equation 8, the specific heat capacity is the sum of an *equivalent* heat capacity (first two terms on the right) and the distribution of latent heat (third term on the right). The latent heat distribution C_L is approximated by:

$$C_L(T) = L \frac{d\theta}{dT} \quad (9)$$

Consequently, the total heat per unit mass released during the phase transformation coincides with the latent heat:

$$\int_{T_{pc}-\frac{\Delta T}{2}}^{T_{pc}+\frac{\Delta T}{2}} C_T(T) dT = L \int_{T_{pc}-\frac{\Delta T}{2}}^{T_{pc}+\frac{\Delta T}{2}} \frac{d\theta}{dT} dT = L \quad (10)$$

The performed FE models are axisymmetric and are constructed over a cylindrical coordinate system with positive z values related to altitudes above sea level (Fig. 4b). Thus, the modelled magma chamber is cylindrical in shape with height h and radius $w/2$. To avoid possible border effects around the reservoir perimeter, we have applied a fillet to the sharp-edged corners (Fig. 4b). The computational domain corresponds to a 40 km (radius) wide section of the crust stretching to a depth of 40 km under the sea level (Fig. 4b). The FE mesh consists of around 110,000 linear triangular elements, with up to 500-metre-size at the host rock and 50 m around the magma chamber – host rock contact (Fig. 4c).

4.2. Physical and thermal properties of the magma and its country rock

The used starting material for the present experiments is the AGV-2 standard andesite (Flanagan, 1967). The andesitic composition (Table 4) is similar to that of the cordilleran batholiths (Castro et al., 2013; Castro, 2014) and, for this reason, experimental results can be applied to magmas involved in crustal processes. The AGV-2 standard composition has been previously chosen as starting material in thermal gradient experiments (Huang et al., 2009).

Taking into account that the possible rapid stages of segregation, ascent and emplacement (Petford et al. 2000) are far beyond the scope of this study, and in order to simplify the model, we assume that magma chamber is instantly filled before the onset of the solidification process. It is considered that the magma is emplaced as totally liquid (Gelman et al., 2013) in a single shot of magma input without further replenishment (Gutierrez & Parada, 2010).

The melt (θ) and solid (ϕ) fractions of the andesitic crystallizing magma are determined by simulations conducted with the Rhyolite-MELTS code (Gualda et al., 2012). Results are reported in the Supplementary Material (Table S1 and S2) and are used as input data in COMSOL. We simulate an isobaric cooling at 500 MPa pressure, and redox conditions one log unite above the quartz-fayalite-magnetite oxygen buffer.

We do not take into account the presence of volatiles, to avoid volume changes and ensure that energy and mass are conserved in phase change models, we consider magma density ρ_{magma} as constant with a value of 2600 kg/m³ assuming a negligible effect of temperature (Gelman et al., 2013). We have tested that the chosen value for ρ_{magma} does not affect substantially the obtained results (Fig. S1; Supplementary Material). For the crust density ρ_{crust} , we assume an average density of 2800 kg/m³ as a good approach for the average composition of a standard continental crust (Turcotte and Schubert, 2002). According to this density value, the centre of the simulated magma chambers reproducing the pressure of the experiments (500 MPa) has to be located between 18.3 and 18.6 km below the surface.

The thermal conductivity of magma k_{magma} and crust k_{crust} is calculated as follows:

$$k_{magma} = \kappa_{magma} \rho_{magma} C p_{magma} \quad (11)$$

$$k_{crust} = \kappa_{crust} \rho_{crust} C p_{crust} \quad (12)$$

With the appropriate subscript, κ , ρ and Cp , corresponding to thermal diffusivity, density and specific heat capacity, respectively. For the magmatic and crustal thermal diffusivity we use the model of Whittington et al. (2009).

To determine the specific heat capacity of the crust, we apply the method of Robinson & Haas (1983) as further modified by Bea (2010):

$$Cp_{crust} = 342 + 1.774 T^* - 1.25 \times 10^{-3} T^{*2} + 3.2 \times 10^{-7} T^{*3} \quad (13)$$

where here T^* refers to the temperature of the crust.

The latent heat L , for silicate phases is estimated to be 400 kJ/kg K. Anyway, the effect of different latent heat value was found to be negligible as demonstrated by some tests where L ranges from 300 to 500 kJ/kgK (Fig. S2; Supplementary Material).

The geothermal gradient of the crust (*thermal_grad*) is fixed at 20 °C/km (Christiensen, 1979; Petford et al., 2000; Tarney and Windley, 1977).

4.3. Boundary conditions

The initial temperature profile for the country rock is defined according to the geothermal gradient and assuming thermal conditions similar to those of Bea (2010). Heat flux is zero through the lateral walls of the country rock (i.e. insulated walls). The heat flow $Q_{mantle} = 0.03 \text{ W/m}^2$ and the surface heat flow $Q_{surface} = 0.07 \text{ W/m}^2$ are assigned to the bottom and top limits of the computational domain (Fig. 4b) (Table 3). For the magma chamber, we assume an initial temperature (T_{0_magma}) equivalent to the *liquidus* temperature provided by Rhyolite-MELTS (1106 °C with 1.2 wt% H₂O).

An example of the performed models is reported as Supplementary Material (COMSOL MULTIPHYSICS commercial software V4.4 or greater is required).

4.4. Numerical modelling results

We have performed simulations considering magma chambers with different sizes and geometries (Table 5). Further geometries were considered, however the results were unsuccessful in establishing a comparison with the experimental data (Table S3). Width (w) and height (h) of the magma bodies have been assigned according to the dimensions of magma chambers in the continental crust (Cruden, 1998; Lipman, 1997; Petford et al., 2000). During cooling, we have extracted, for each time step, the magma temperature along the A-A' profile (Fig. 4b) until the temperature in the innermost portion of the chamber decreases 1 °C (the estimated error from the temperature measure by thermocouples) from the AGV-2 *liquidus* (i.e. 1106 °C) to 1105 °C. At this temperature, we consider the interior of the magma chamber to be just below $T_{liquidus}$. Time steps for the different models vary from 0.08 to 1.6 ka depending on the size of the simulated magma chamber, the larger steps corresponding to the larger reservoirs.

On the whole, we observe that the cooling time, evolution and shape of the thermal profiles at different time steps depend mainly on the magma chamber volume and aspect ratio (Fig. 5). Thus, for approximately the same reservoir volume (e.g. case studies 12 and 17), the cooling process will be more efficient as the aspect ratio decreases. Similarly, the thermal gradient from the walls to the centre of the magma chamber will be steeper according to lower magma chamber aspect ratio (e) (i.e. sill-like reservoirs) (Fig. 5).

5. Comparison between experimental and numerical results

5.1. Methodology

In order to compare the results obtained between numerical and experimental results, it is required to normalize the distances across both thermal profiles. On one hand, we have normalized the distance along the A-A' profile by $w/2$ (Fig. 6a) for the numerical runs. On the other hand, for experimental (double thermocouple) results, we have normalized the distance of the measure position (r_{exp_i}) for each experimental temperature measurement (T_{exp_i}) with respect to the standard length ($d_{exp}=10$ mm) of the entire capsule (Fig. 6b). Therefore, the positions along the thermal gradients from numerical profiles, after normalization, can be compared with those from experimental data. The positions along the experimental thermal profile and the central axis of the magma chamber were calculated according to the entire capsule length and to the magma chamber radius. The best-correlated examples have been selected for the comparison.

Although in thermal gradient experiments the temperature ranges from liquidus to solidus, it is not known what portion and/or evolutionary stage of a given magma chamber is reproduced by the experimental thermal gradient (Fig. 7a). For example, the normalized capsule length (d_{exp_nor}) may correspond to the half width of a magma chamber ($w/2$), consequently, the temperature values of our experiments (T_{exp}) cover the entire A-A' thermal profile (see the first diagram in Fig. 7b). Thus, the values of T_{exp} located at $r_{exp_i_nor}=0$ will be at position A —the centre of the magma chamber— and the values of T_{exp} at $r_{exp_i_nor}=1$ at A', the magma chamber-host rock interface (Fig. 7b). Alternatively, d_{exp_nor} may match only a portion of the A-A' profile. In this case, the maximum and minimum temperatures will be shifted from the centre or walls of the magma chamber by a given magnitude (*offset*). In order to describe the latter situation, we define the position ($r_{exp_i_nor}$) of the experimental temperature values along the A-A' profile as follows (Fig. 7a):

$$r_{exp_i_scaled} = r_{exp_i_nor} \cdot scale + offset \quad (14)$$

where the variable *scale* is a scale factor (ranging from 0 to 1) for the total distance (d_{exp_nor}) between the centre of the furnace and the most distant measure position corresponding to the lowest temperature. The *offset* indicates the position in which the experimental points are located along the A-A' profile with respect to the centre of the chamber. This parameter is a consequence of the fact that *scale* is lower than 1; i.e. the experimental points do not cover the entire thermal profile of the magma chamber, but only a limited portion. Thus, for $scale < 1$, the experimental data set does not start from the centre of the magma chamber but at a certain distance from it. This distance is defined as *offset* (Fig. 7a):

$$offset \leq 1 - d_{exp_nor} \cdot scale \quad (15)$$

A limiting factor is that the farthest experimental point has to be inside the magma chamber or in contact with the host rock (Fig. 7a and b).

A priori we do not know the *scale* and *offset* values that will lead to a better fit of the experimental measurements with the numerical thermal profiles. Thus, for each A-A' thermal profile obtained with the numerical runs, we have compared the experimental values using different *scale* and *offset* values from 0 to 1 and from 0 to $1 - d_{exp_nor} \cdot scale$, respectively. Then, for each experimental data we have calculated the error percentage between the temperatures predicted by the model and those observed as follows:

$$err = \frac{T_{exp_i} - T_{num_i}}{T_{exp_i}} 100\% \quad (16)$$

We consider that the best fits between the experimental values and the numerical data are those *scale* and *offset* pairs that accomplish the following points:

- 1) The error for the first experimental point is less than 1% ($err_1 < 1\%$) (i.e. the temperature difference between the experimental value and the numerical

one, $T_{exp_i} - T_{num_i}$, is <11 °C). In this way we ensure that the modelled magma in the numerical models is still almost fully liquid as occurs within the experimental capsule.

- 2) The error in the second experimental point is below 5% ($err_2 < 1\%$) (i.e. $T_{exp_i} - T_{num_i} < 45.5^\circ\text{C}$). The fit between T_{exp_i} and T_{num_i} is heavily dependent on the position along the A-A' profile because of the steep slope of the thermal gradients implying that small differences in $r_{exp_i_scaled}$ involve large temperature changes. For this reason, a higher err value is allowed in the second experimental point.
- 3) The estimated err in the experimental point closer to the country rock contact is below 10% ($err_3 < 10\%$) (i.e. $T_{exp_i} - T_{num_i} < 73.2$ °C). Since the modelled temperature close to the country rock contact may be influenced by a number of parameters (e.g., the thermal gradient of the host rock), we consider that the error cannot be easily reduced, due to we have a wide range of options in nature that cannot be addressed in full in this study.

Thus, we consider as best fitting models those where it is possible to find *scale* and *offset* pairs that fulfil the points imposed above. The second best fitting group of models are those where the *scale-offset* pairs calculated lead to $err_1 < 1\%$, $err_2 < 7.5\%$ and $err_3 < 12.5\%$. Above these error values we consider that the numerical models fail to reproduce the thermal gradient obtained in the experiments and that there is no significant equivalence between them.

We estimate the final deviation between experimental and numerical data (Δ) using Root-Mean-Square Error (RMSE) as follows:

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (T_{exp_i} - T_{num_i})^2}{n}} \quad (17)$$

where n is the total number of the experimental points, in this case $n=3$, and T_{num_i} is the temperature predicted by the numerical simulation at the position $r_{exp_i_scaled}$. The RMSE is a common measure of the difference between values predicted by a model and those observed. Taking into consideration the restrictions mentioned above regarding the values allowed for err , the best fitting models will have a $RMSE < 50.15^{\circ}\text{C}$ and the second group $< 66.4^{\circ}\text{C}$.

5.2. Comparison results for an andesitic magma at 500 MPa

Our results are illustrated in Figs. 5 and 8, and the best *scale* and *offset* values are listed in Table 6. The minimum final deviation ($RMSE$) for each case study is illustrated in the Supplementary Material (Fig. S3). It is clear from the results that the temperature difference increases as the aspect ratio decreases (Fig. S3). The best fitting models are those with larger aspect ratio (e.g. Case studies 13, 14, 15).

An important result from this study is that as the aspect ratio of the magma chamber increases, a greater *scale* value is required to obtain the best correspondence between the experimental and numerical results (Fig. 8a). These case studies have long time intervals, reaching 100 ka (Fig. 8b).

In other words, the time interval, within which the experimental points (T_{exp}) fit their equivalent in the numerical thermal profiles, increases proportionally with scale and aspect ratio.

This observation indicates that in the case of sill-like reservoirs, the experimental thermal gradient corresponds to a small fraction of the magma chamber, i.e. small-scale values. Additionally, for reservoirs with low aspect ratios, the experimental profiles correspond to short time windows (Fig. 8b) and the final temperature deviation reaches greater values (Fig. S3). Examples with extremely low values of aspect ratio do not

reach adequate fits for the experimental measurements (e. g. case study 4 and 18, labelled in black in Fig.5).

On the other hand, when the height is > 5 km (2, 14, 15 and 17), the predicted time interval is high, ranging from 60 to 120 ka (Fig. 5). A larger fraction of the cooling magmatic body will be represented by the experimental points for magma bodies with $h \approx w$ (i.e. e close to 1) (Fig. 5).

In most cases, the offset value is close to $1 - d_{exp_nor} \cdot scale$ (Table 6). This indicates that temperature data (T_{exp}) fit quite well with the numerical results that encompass the contact between the magma chamber and its host rock when $r_{exp-scale} = 1$.

The time frame is the time interval for which experiments and numerical simulations match with each other. We observe three distinct trends that correspond to the different e/V ratios of the simulated reservoir (Fig. 8b), where V is the volume of the modelled magma chamber assuming a cylindrical shape of radius $w/2$, and e is the aspect ratio (h/w). This e/V relation indirectly illustrates the heat loss efficiency, being higher in sill-like intrusions (low e) compared to spherical ones ($e=1$). The selected combinations of h and w yield three different e/V categories or cases (Fig. 8b). For those cases sharing e/V ratio, the time window of good match increases with the aspect ratio (Fig. 8b). Thus, small sill-like magma reservoirs (e.g. case study 13, $V = 392.7 \text{ km}^3$; e/V ratio = $1.3 \times 10^{-3} \text{ km}^{-3}$) will be related to the same time window than large magma volumes with e values close to 1 (e.g. case study 11, $V = 3534 \text{ km}^3$; e/V ratio = $4.7 \times 10^{-5} \text{ km}^{-3}$). For the same $e \approx 1$ value, large reservoirs will lead to experimental values fitting in a time window wider than that of small magma chambers. Thus, the time window in which the experimental values fit the numerical results will be lower than a few thousand years (e.g. 19) or over 120 ka (e.g. case study 2) spreading over two orders of magnitude, depending on each case study.

In summary, keeping constant other variables such as depth or magma/crust thermal properties, the geometry and size of the magma chamber appear to be the most important parameters controlling the evolution of cooling. The higher deviation values arise when comparing the temperature at the contact with the host rock and the minimum temperature measured within the experimental runs. The temperature at the contact with the host rock exceeds the minimum temperature of the experimental measurements (732 °C). The AGV-2 *solidus* is around 680 °C (Table S2) but the temperature is higher than this value due to the imposed geothermal gradient (20 °C/km) and the influence of the latent heat (Fig. S2). Consequently, high deviation values come from this initial temperature difference.

6. Discussion and conclusions

Results obtained in this study show how thermal gradient experiments can reproduce the natural systems over the effects of a short time scale and limited dimensions.

The scaling factor provides the portion of magma chamber represented by the experimental thermal gradient (Fig. 8). In all cases, the represented fraction is found next to the contact with the host rock. During early stages corresponding to the beginning of magma chamber cooling, the temperature change is constrained to a reduced space next to the host rock. Due to the fact that the thermal profile used for the comparison was chosen as a function of the *liquidus* temperature of the starting melt composition, the outputs from the scaling correspond to these initial stages, for which the thermal gradient is very steep and is constrained to the area near to the host rock contact. In fact, the most of the decoupling between experimental and numerical data (Δ

in Fig. S3) are reached at the contact. This is because the dwell time is not enough to solidify completely the magma at the contact with the host.

The thermal gradient experiments mostly reproduce the sill-like magma chambers for short periods of time or thicker magma chambers for longer periods of time (Fig. 5). Thin magma bodies with low aspect ratio will experience fast cooling, due to heat loss in their roof and footwall. Magmatic systems, with vertical dimensions smaller than 5km, are not able to reduce the sharp temperature change, imposed by the thermal contrast with the host rock. Therefore, the maximum temperature of the magma (1106 °C, AGV *liquidus*) decreases rapidly at the initial stage of cooling. As a consequence, the experimental measurements (fixed at the AGV *liquidus*) cannot be compared with the modelling results obtained at the final stage of magma chamber evolution for periods of time > 20 ka.

By contrast, it can be argued that thick magma chambers can maintain the *liquidus* in the innermost parts for a long time (Fig. 5). Thereby, the experimental thermal profiles are comparable to the numerical modelling during longer time intervals, with a maximum duration of 120 ka (Fig. 8).

In summary, the portion of the thermal profile represented by the experimental capsule may range from 0.1 to 0.5 of the radius of the magma chamber depending on volume and aspect ratio.

For those examples using a low aspect ratio up to 0.1, we found it matched the experimental modelling (Fig. 5). However, the represented portion varies only from 0.1 to 0.2 (Fig. 8a), since the space between the *liquidus* and *solidus* is small. For these examples, the melt fraction is high and the thermal gradient exhibits a steep behavior with respect to the other case studies. When the thermal gradient diminishes in magma

chambers with these geometries, the temperature at the core is low than the AGV *liquidus* and therefore, the comparison is not possible.

The scaling factors can be used for experiments with similar temperatures at the hotspot zone that, in turn, control the thermal profile in the assembly of the piston-cylinder. Since the experimental thermal profiles show a similar pattern for temperatures measured next to the hotspot, the scaling factor can be applied to thermal-gradient experiments at 500 MPa and over temperature range between 1200 and 1000 °C. Experimental thermal gradients for different pressure and temperature conditions, simulate distance and cooling stages that can be calculated through our approach. In both cases, the thermal gradients become smoother as the cooling proceeds.

6.1. Implications

Processes occurring in deep-seated magma chambers are partly responsible for the style of explosive or effusive eruptions and their understanding is essential in volcanology. An important implication of our comparative study is the establishment of the range of magma chamber geometries and volumes for which thermal gradient experiments can be represented, within the limits imposed using the scaling factors proposed in this study. Thermal gradient experiments are able to reproduce the solidification front (Marsh, 2002) including the whole temperature range from *liquidus* to *solidus*.

Magma chambers volumes represented by thermal gradient experiments range from 150 to 3500 km³ (Fig. 8b). The contexts of application for these crystallization experiments at 500 MPa are representative of typical dimensions of batholith-like, large silicic magma bodies (Lipman, 2007; Scandone and Acocella, 2007; Petford et al., 2000) and small silicic plutons.

Furthermore, batholiths are typically characterized by tabular geometries with thickness not exceeding 5 to 10 km (Elo and Korja, 1993; Petford et al., 2000). These low-aspect ratio bodies are the geometries most suitable for the comparison between modelled thermal gradients and experiments. According to Cruden (1998), tabular granites can be quickly emplaced despite the geometry changes in thickness during emplacement. Structural and geophysical surveys support low aspect ratio and sill-like geometries with depth feeder zones (Ameglio et al., 1997; Ameglio and Vigneresse, 1999). The incremental growth of magma reservoir during various steps over protracted periods has been also recorded (Annen et al., 2006).

On a different note, the time frame during which the experimental-numerical comparison is possible (Fig. 8b) corresponds to time scales for differentiation to high-silica magmas (Hawkesworth et al., 2000; Hawkesworth et al., 2004).

It is widely accepted that large magma chambers have low aspect ratios. Results from thermal modelling simulating magma chambers with a small height and great width closely match with thermal profiles obtained in laboratory. This means that thermal gradient experiments can be successfully applied to batholiths, small silicic plutons and super volcanoes magma chambers (Fig. 5).

Our results are related to this specific case study for andesitic compositions; however, the methodology can be applied to other compositions and additional experimental results.

Figure captions

Figure 1. Sketch illustrating thermal gradient experiments that may represent varied evolutionary stages of the same magma chamber. (a) The experimental thermal gradient

may correspond to early stages of cooling, representing just a distance of 2 km from the boundary with the host rock. (b) In a more evolved magmatic system, the thermal gradient imposed to the experiments can be equivalent to a distance of 5 km from the walls of the magma chamber (red zone).

Figure 2. Design of the experimental assembly showing the desired measure thermocouple positions (MP1 and MP2) in both CG1 and CG2 runs. The control position called CP marks the thermocouple located into the hotspot.

Figure 3. Temperature measurements at 6.6 mm (a) and 10 mm (b) from the centre of the furnace (hotspot) showing the response to temperature changes at the control position (hotspot). Regression curves are also represented.

Figure 4. (a) Example of a thermal profile. (b) Sketch of the numerical models set-up also showing the used boundary conditions. (c) Example of the Finite Element mesh used for the modelling.

Figure 5. Magma chamber temperatures along the A-A' profile obtained by numerical modelling. For illustrative purposes, a sketch of the modelled magma reservoir is also included. Black diamonds and yellow squares represent the experimental values considering the maximum and minimum *scale*, respectively. Errors of temperature are less than the vertical length of the symbols. Errors of the *offset* and *scale* values are represented for each experimental point (black bars). Best and second best fitting models are indicated with green and yellow colour, respectively. *ns*: Drawings of magma chambers are not scaled, only aimed to illustrate the aspect ratio.

Figure 6. Procedure developed to compare experimental and numerical results. (a) Normalization of the positions along the numerical thermal profile (A-A') relative to magma chamber radius ($w/2$). (b) Normalization of measured (experimental) positions (r_{exp_i}) according to the standard capsule length (10 mm).

Figure 7. (a) Comparison between numerical and experimental thermal profiles, after normalization and the processing of the experimental data through the use of *scale* and *offset* parameters. (b) Example of situations after data processing by applying scale and offset parameters.

Figure 8. Diagrams of the scaling results from the comparison between numerical modelling and experimental data. (a) Aspect ratio ($e = height/width$) vs. scale (simulated distance/radius of the magma chamber) plot reveals the influence of geometry on the distance simulated by the experimental thermal profiles (b) Aspect ratio vs. maximum age diagram showing the simulated time frame of the magma chambers for each case study. Magma volume is indicated (black lettering) and the black arrow marks the volume increase. Dashed lines mark magma chamber groups with equal e/V ratio (blue dashed line for $4.7 \times 10^{-5} \text{ km}^{-3}$, black dashed line for $2 \times 10^{-4} \text{ km}^{-3}$, red dashed line for $1.3 \times 10^{-3} \text{ km}^{-3}$).

Figure S1. Diagram showing the influence of the magma density on the thermal profile along the central axis of the magma chamber (A-A' profile). The time and magma chamber geometry selected for these thermal profiles are taken arbitrarily.

Figure S2. Plot of normalized distance vs. magma temperature displaying the influence of the latent heat on the thermal profiles along the central axis of the magmatic system (A-A' profile).

Figure S3. Aspect ratio vs. deviation diagram showing the dependence of the decoupling between numerical and experimental results according to the geometry of the magma chamber.

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Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8

Table 1

Experimental conditions

Run	CG1	CG2
Location of the measure thermocouple (mm)*	6.6	10
Initial temperature (°C)	1200	1200
Final temperature (°C)	950	800
P (MPa)	500	500
Cooling ramp (°C/hour)	10	10/0.6

* Distance from the centre of the furnace (hotspot)

Table 2

Temperature values at different distances

Run n° (reference)	CG1/CG2	CG1	CG2
Distance from the centre of the furnace (mm) ($r_{exp,i}$)	0	6.60	10.00
Normalized distance (position/ total length) ($r_{exp,i,nor}$)	0	0.66	1.00
Temperature (°C)	1106	909.1	732.3

Table 3

Physical and thermal parameters

Symbol	Value	Variable	SI Unit
α		Phase change smoothed function	-
C_p		Specific heat capacity at constant pressure	J/kg°C
$C_{p_{crust}}$	Eq. 10	Specific heat capacity of crust ¹	J/kg°C
$C_{p_{melt}}$	Supp. Mat. Table S2	Specific heat capacity of magma (melt phase)	J/kg°C
$C_{p_{solid}}$	Supp. Mat. Table S2	Specific heat capacity of magma (solid phase)	J/kg°C
d	18.3-18.6	Magma chamber depth	km
e	0.1-1	Magma chamber aspect ratio	-
h	2-10	Magma chamber height	km
κ_{magma}	$f(T)$	Magma thermal diffusivity ²	m ² /s
κ_{crust}	$f(T)$	Crust thermal diffusivity ²	m ² /s
k		Thermal conductivity	W/m°C
k_{magma}	Eq. 8	Magma thermal conductivity ²	W/m°C
k_{crust}	Eq. 9	Crust thermal conductivity ²	W/m°C
L	400	Latent heat of crystallization ¹	kJ/kg
θ	Supp. Mat. Table S1	Melt fraction ³	-
Q_{crust}	Eq. 11	Heat production crust ¹	-

Q_{mantle}	0.03	Subcrustal heat flow ¹	W/m ²
$Q_{surface}$	0.07	Surface heat flow ¹	W/m ²
ρ_{crust}	2800	Crust density	kg/m ³
ρ_{magma}	2600	Magma density	kg/m ³
ϕ	1- θ	Solid fraction ³	-
$thermal_grad$	20	Crustal thermal gradient	°C/km
$T_{liquidus}$	1106	Magma liquidus temperature ³	°C
$T_{solidus}$	676.4	Magma solidus temperature ³	°C
$T_{surface}$	20	Surface temperature	°C
T_{0_magma}	1106	Initial magma temperature	°C
T_{0_crust}		Initial crustal temperature	°C
P	500	Magma chamber internal pressure at $h/2$	MPa
w	10-30	Magma chamber width	km

1, Bea (2010); 2, Whittington et al. (2009); 3, use Rhyolite MELTS code by Gualda et al. (2012)

Table 4
Composition of the starting material
used for the simulation

Major elements (wt%)	AGV-2
SiO ₂	59.30
TiO ₂	1.05
Al ₂ O ₃	16.91
FeO	6.08
MgO	1.79
MnO	0.00
CaO	5.20
Na ₂ O	4.19
K ₂ O	2.88
P ₂ O ₅	0.48

Table 5

Case studies used for the numerical modelling of magma chambers

Case study	2	3	4	11	12	13	14	15	16	17	18	19	20
Width w (km)	20	20	20	30	30	10	10	10	20	20	30	10	10
Height h (km)	10	5	2	5	3	5	7	10	3	7	2	2	3
Volume V (km ³)*	3142	1571	628.3	3534	2121	392.7	549.8	785.4	942.5	2199	1413	157.1	235.6
Aspect ratio e (h/w)	0.50	0.25	0.10	0.17	0.10	0.50	0.70	1.00	0.15	0.35	0.07	0.20	0.30

* Volume calculated assuming cylindrical shapes

Table 6

Results from numerical runs for the time frame, scale and offset values

Case study	<i>Time frame</i> (ka)	<i>scale</i>	<i>scale</i> $\times$ w/2 (km)	<i>offset</i>	<i>offset</i> $\times$ w/2 (km)
2	0.07-120.5	0.015-0.36	0.15-3.60	0.638-0.985	6.375-9.85
3	0.07-31.10	0.015-0.17	0.15-1.70	0.838-0.985	8.375-9.85
4	0.07-4.80	0.015-0.06	0.15-0.60	0.948-0.985	9.475-9.85
11	0.07-22.80	0.013-0.09	0.20-1.35	0.908-0.987	13.625-14.80
12	0.07-9.90	0.013-0.06	0.20-0.90	0.938-0.987	14.075-14.80
13	0.07-30.10	0.03-0.34	0.15-1.70	0.660-0.97	3.30-4.85
14	0.13-63.42	0.04-0.50	0.20-2.50	0.50-0.96	2.50-4.8
15	0.07-63.10	0.03-0.50	0.15-2.50	0.50-0.97	2.50-4.85
16	0.07-11.30	0.015-0.10	0.15-1.00	0.898-0.985	8.975-9.85
17	0.07-59.98	0.015-0.24	0.15-2.40	0.758-0.985	7.575-9.85
18	0.07-4.80	0.013-0.05	0.15-0.75	0.948-0.99	14.22-14.85
19	0.00-3.8	0.02-0.14	0.10-0.70	0.86-0.98	4.30-4.90
20	0.00-10.62	0.03-0.14	0.15-0.70	0.86-0.97	4.30-4.85

Graphical abstract

Highlights

Experimental thermal gradients simulate transient stages of cooling magma chambers.

Numerical modeling approaches the scaling of crystallization experiments.

Experimental thermal gradients are comparable to sill-like magma chambers.