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PII: S0895-9811(20)30394-1

DOI: https://doi.org/10.1016/j.jsames.2020.102851

Reference: SAMES 102851

To appear in: *Journal of South American Earth Sciences*

Received Date: 27 May 2020

Revised Date: 24 August 2020

Accepted Date: 25 August 2020

Please cite this article as: Cristallini, E., Sánchez, F., Balciunas, D., Mora, André., Ketcham, R., Nigro, Joaquí., Hernández, J., Hernández, R., Seamless low-temperature thermochronological modeling in Andino 3D, towards integrated structural and thermal simulations, *Journal of South American Earth Sciences* (2020), doi: https://doi.org/10.1016/j.jsames.2020.102851.

Ernesto Cristallni: Conceptualization, Methodology, Software coding, Writing- Original draft preparation and figures, Investigation, cross section construction. **Francisco Sanchez.**: Conceptualization, Methodology, Software coding, Writing- Original draft preparation, Investigation. **Daniel Balciunas**: Software coding. **Andres Mora**: Reviewing and Editing.**: Richard Ketcham**: Software coding, Investigation, Validation.: **Joaquín Nigro:** Software coding, **Juan Hernández:** Writing- Reviewing and Editing, field work and geology, **Roberto Hernández:** field work and geology, cross section construction, Funding acquisition.

Seamless low-temperature thermochronological modeling in Andino 3D, towards integrated structural and thermal simulations

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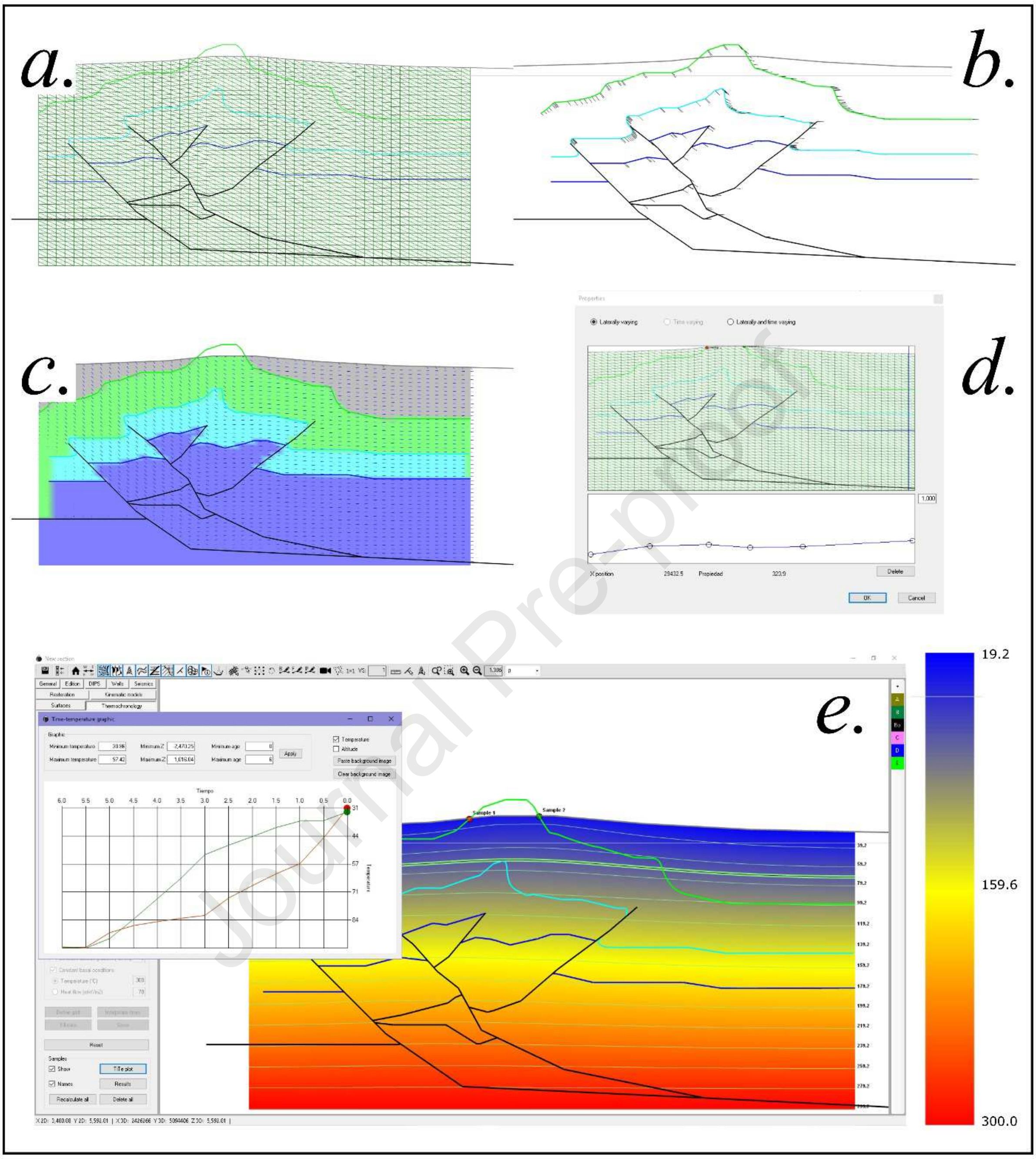
Abstract

We present the development of thermochronological tools for Andino 3D® software, that integrates Fetkin (Finite Element Temperature Kinematics). These tools allow the user to work on both the structural and the thermochronological model at the same time, providing a user-friendly environment that overcomes the need to work with different programs. Thermochronological and structural models can be checked and eventually corrected in a visual and intuitive form by following a 4-step workflow. The first step of such workflow is to define the thermochronological computing grid, checking in real time, if the resolution and coverage are satisfactory. After that, the interpolation process can be done, whereby velocity vectors for all nodes in beds and faults are calculated for all interpolated times. The third step of the workflow consists of filling thermal properties and velocities for all grid cells. The final step is the calculation of the thermal state at each time in the reconstruction. Boundary conditions (basal temperature, basal heat flow, surface temperature and altitude gradient) are defined by mouse picking as constant, spatially varying, time varying or spatially and time varying. To check the feasibility of a structural model, thermochronological samples can be defined at desired positions to predict time-temperature variations. Simulated fission track ages, mean track lengths and age standard deviations can be calculated for different minerals (apatite and zircons). Also, cooling ages and %Ro can be simulated for (U-Th-Sm)/He and vitrinite systems, respectively. The Carohuaicho structure in the southern Bolivia sub-Andean Ranges is presented as a case of study to demonstrate these tools. Andino 3D® allowed us to successfully simulate the t-T paths of four samples where (U-Th-Sm)/He measurements were available. The different models performed permitted us to conclude that a low geothermal gradient was likely to be present during the last 7 Ma of Andean deformation in the study region.

Introduction

Structural and thermochronological modelers often face the challenge of working with different programs and computational codes to reproduce a feasible multidimensional thermochronological model. In addition, most such programs and codes require the modeler to do some scripting, thus diverting attention from where it is required. The new version of Andino 3D® software allows the user to work on both the structural and the thermochronological model at the same time, thus providing a user-friendly environment that overcomes the need to work with different programs.

Andino 3D® is a structural modeling software developed by LA.TE. ANDES thermochronological laboratory (Argentina) with capabilities to work in 2D and 3D models, connecting both views simultaneously. Its graphical interface facilitates working with balanced cross sections and kinematic modeling. Here we present the integration of thermochronological tools for Andino 3D®, following the previous development of Fetkin (Finite Element Temperature Kinematics), a software for forward modeling of thermochronological ages (Almendral et al, 2015). Developed by Ecopetrol (Colombia), Fetkin was designed to work with cross sections constructed using third-party software (Castelluccio et al, 2015; Mora et al, 2015). By taking advantage of Andino 3D's graphical interface, the Fetkin-Andino 3D integration provides the user an all-in-one program where thermochronological and structural models can be checked and eventually modified in real-time in a visual and intuitive form.



X position 28432.5 Propiedad 323.9

Minimum temperature 30.86
Maximum temperature 57.42
Minimum Z 2,470.25
Maximum Z 1,016.04
Minimum age 0
Maximum age 6
☑ Temperature
☐ Altitude

Figure 1: The Andino 3D$^{®}$ thermochronological workflow is divided into four processes to allow users to check each step and make any necessary corrections to their structural model. ***a.*** Definition of the thermochronological computing grid. The grid can be visualized, checked and modified in real time until resolution and coverage are satisfactory. ***b.*** Interpolation process, where the structural reconstruction is interpolated in any number of regular time steps (see *Figure 2*). In this process, the velocities for all nodes in beds (i.e. horizons or layers) and faults are calculated for all interpolated times (see little segments in the figure, depicting velocity vectors). ***c.*** Filling of thermal properties (thermal conductivity, heat capacity), density, and velocities for all grid cells. Colors in the figure represent the thermal properties and little blue

segments the velocities. ***d.*** All types of upper and lower boundary conditions are permitted, allowing the user to easily test (mouse picking) different geological hypotheses. **e.** Computing the thermal state at each time in the reconstruction (see *Figure 2*). Isotherms can be plotted, and synthetic samples can be defined to check the feasibility of a structural model and to predict time-temperature variations at particular locations (in the example red and blue curves are time-temperature variations for two different samples).

Andino 3D® allows structural restoration either by using kinematic algorithms or by drawing “by hand” with traditional structural techniques. If a structural model is performed in third-party software, Andino 3D® also allows various file type options for importing section data. Once the geometries for each time step in the studied reconstruction are defined, the thermochronological workflow can be started. This workflow is divided into four processes (Figure 1), to allow users to check each step and eventually make any necessary corrections to their structural model. The first step in the workflow is to define the thermochronological computing grid (Figure 1a). After defining a grid, the user can immediately visualize it and check, in real time, if the resolution and coverage are satisfactory. After that, the interpolation process takes place (Figure 1b and Figure 2). Andino 3D® will interpolate the structural reconstruction in any number of regular time steps (Figure 2), as requested by the user. In this process the velocity vectors for all nodes in beds (i.e. horizons or layers) and faults are calculated for all interpolated times (Figure 1b). Structural balancing deficiencies might be evidenced by unsatisfactory velocity interpolation, and can be corrected by refining the kinematic sequence. After this, the third step of the workflow can start, and thermal properties and velocities are filled for all grid cells (Figure 1c). This is the more time-consuming process for the computer processor and it may take on a conventional desktop computer (Intel i5 dual core, for example) from seconds to minutes, depending on the grid dimension and number of time steps interpolated. In the same way as in previous steps, the user can check the quality of this filling, and eventually go back and make corrections to the model. The last workflow step is the computing of the thermal state at each time in the reconstruction (Figure 1e and 2b). For this, boundary conditions are defined easily using the mouse (Figure 1d). The program allows constant, spatially varying, time varying, or spatially and time varying boundary conditions (both upper and lower).

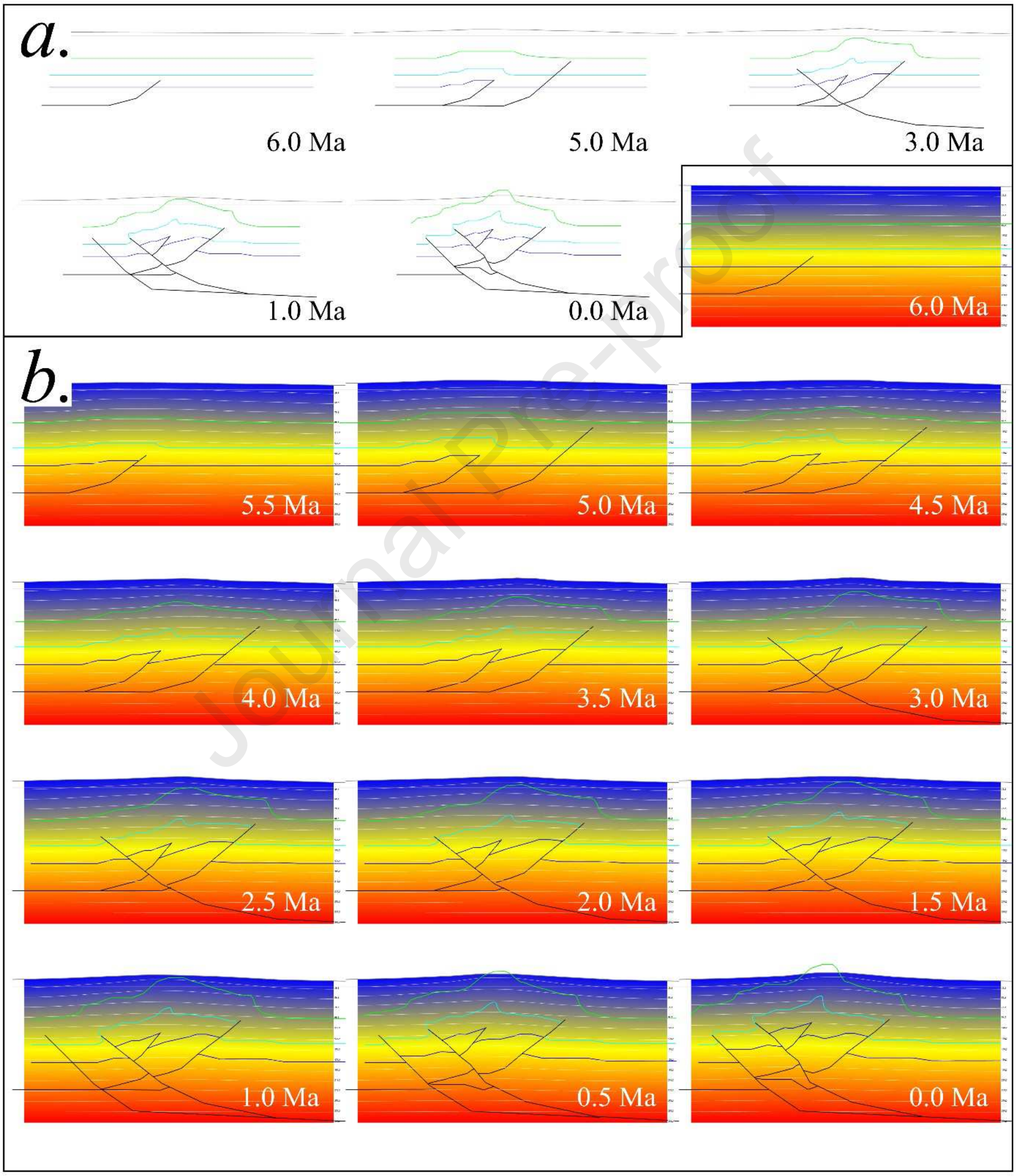


Figure 2: a. Input structural model developed using kinematic modeling tools in Andino 3D® (five sections were constructed for different times, 6 Ma, 5 Ma, 3 Ma, 1 Ma and 0 Ma). ***b.*** Resulting interpolated sections with thermal state calculated. Interpolation was done in 0.5 Ma time steps resulting in thirteen sections. Thermal evolution of the model is complete.

Furthermore, basal temperature, basal heat flow, surface temperature and altitude gradient can be changed in this way (mouse picking). Such flexible boundary conditions provide the user the opportunity to study geological settings such as McKenzie rifting models, where heat input from the ascending asthenosphere is known to evolve in time.

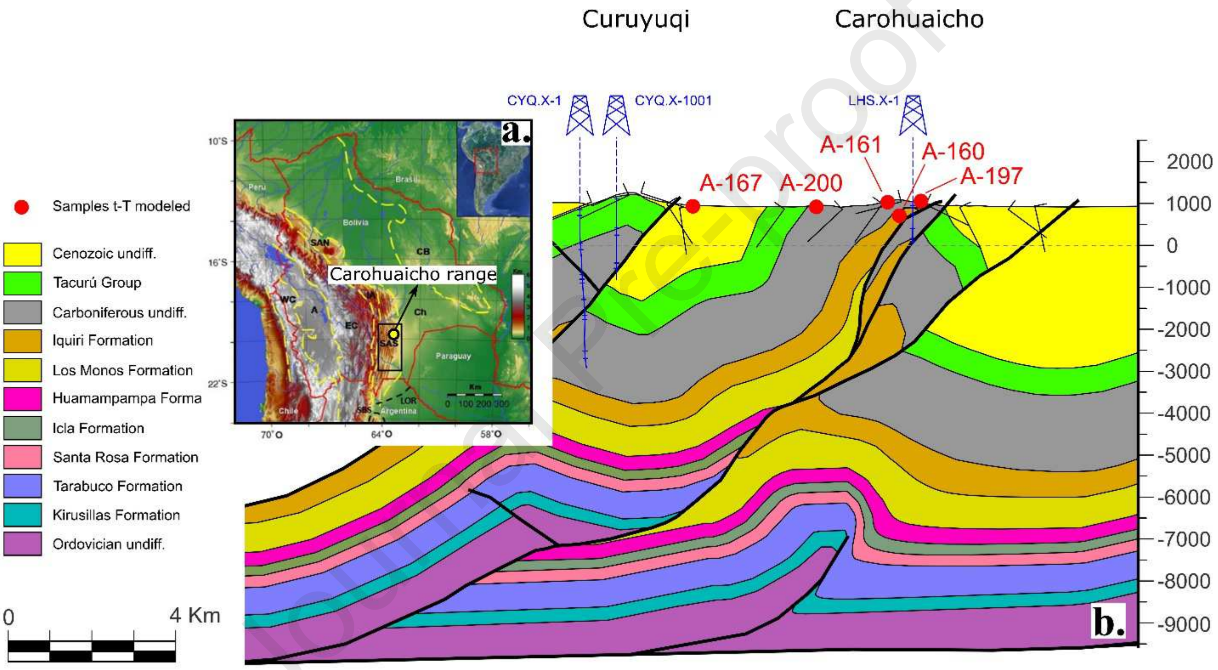


Figure 3: a. Location of the Carohuaicho structure (yellow circle) in the southern sub-Andean Ranges (black rectangle) in southern Bolivia. ***b.*** Structural cross section modified from Hernández et al. (2020, this volume). The samples used to compare with Andino 3D® simulation are shown.

To check the feasibility of a structural model, thermochronological samples can be defined at desired positions to predict time-temperature variations (Figure 1e). Samples do not necessarily have to be located on bed boundaries, thus they can be defined anywhere in the model. Simulated fission track ages, mean track lengths and age standard deviations can be calculated for different minerals (apatite and zircons) for the fission track system. Cooling ages and %Ro can be simulated for (U-Th-Sm)/He and vitrinite systems, respectively. We remark that thermochronological computations run very quickly, with the whole process taking from some minutes up to one hour (for very dense grids and/or hundreds of interpolation times).

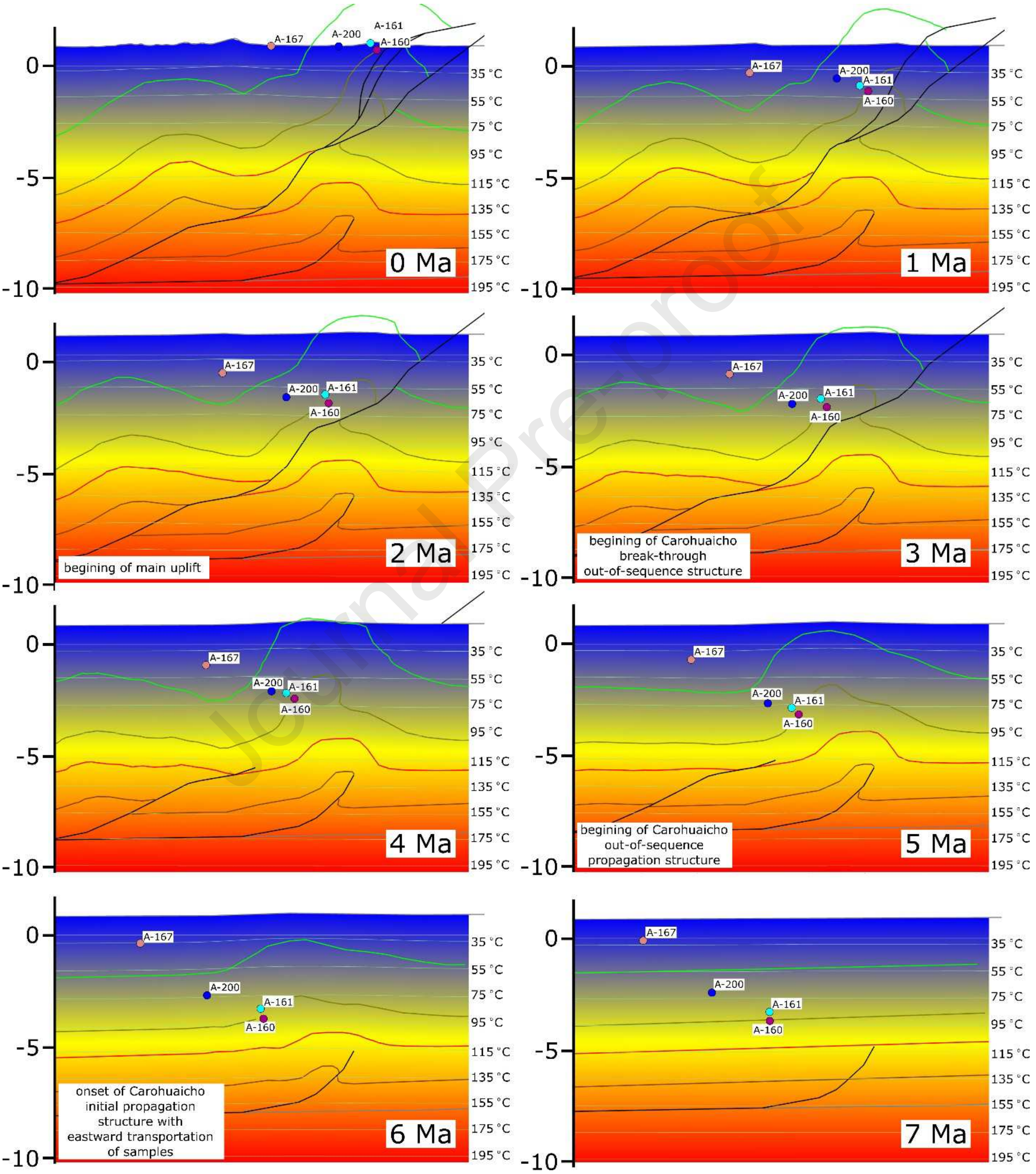


Figure 4: Thermal evolution of the Carohuaicho anticline. Originally, eleven cross sections were constructed as input for this model to represent structural evolution of the Carohuaicho range (see text). They were constructed combining kinematic forward modelling and traditionally “by hand” section construction/restoration methods. To obtain a precisely resolved kinematic history, 70 sections were interpolated in Andino 3D® from the original eleven, each one every 100 ka. Only 8 of them are shown for simplicity in this figure. Stratigraphic references are in Figure 5. Basal temperature: 200°C; surface Dirichlet-type boundary condition: 20°C; atmospheric cooling rate: 5°C/Km.

Case of study: Carohuaicho structure

To test the operation of the thermochronological module of Andino 3D®, the Carohuaicho anticline, in the southern sub-Andean Ranges of Bolivia, was considered (Figure 3). Four samples (A-167, A-200, A-161 and A-160; see Fig. 3) analyzed with the (U-Th-Sm)/He in apatite technique (see Hernandez et al., 2020; this volume) were used to understand the evolution of the system after the main deformational episode, which took place at 7 Ma. Such deformational activity, linked to the Andean orogeny (Mingramm et al., 1979; Baby et al., 1997; Kley and Monaldi, 1999; Hernández et al., 2002; Hernández et al., 2020), was responsible for more than 50 km of shortening related to the east-verging thin-skinned thrust belt of the sub-Andean system in Bolivia and northwestern Argentina. The Carohuaicho anticline sits between the Curuyuqui and Borebigua structures, and constitutes a complex break-through fault propagation fold formed by a succession of Devonian, Carboniferous, Mesozoic and Cenozoic rocks. Details of the regional geology and structure can be found in this same volume by Hernández et al. (2020).

Units	Rock types	Density Kg/m^3	Thermal conductivity W/(m °K)	Caloric capacity J/(kg °K)
Cenozoic units	Sandstones and shales	2760	2.5	865
Tacurú + Carboniferous units + Iquiri	Sandstones and shales	2780	2.6	850
Los Monos	Shales and sandstones	2710	2.3	860
Huamampampa + Icla + Santa Rosa + Tarabuco	Quarcites, sandstones and shales	2780	2.6	850
Kirusillas + Ordovician	Shales and sandstones	2710	2.3	860

Table 1: Density and thermal properties used for simulation in Andino 3D®.

A kinematic reconstruction since the onset of the Cenozoic deformation, at 7 Ma, was performed. Eleven (11) balanced structural sections were obtained (combining kinematic forward modeling and traditionally “by hand” section construction/restoration methods) considering the deformational history described by Hernández et al. (2020, see for further details). Such deformational history mainly consisted of an initial pulse of deformation between 7 and 6 Ma and, since 3 Ma, an acceleration of uplift with the development of out-of-sequence structures. To obtain a finely resolved kinematic history, 70 sections were interpolated in Andino 3D® from the original eleven, each one every 100 ka; however, only 8 of them are shown for simplicity (see Fig. 4). To account for lithological variations in the temperatures to be modeled, a simplified stratigraphy (Fig. 5) was reproduced after Hernandez et al. (2020, this volume). Table 1 shows the lithological composition and thermal properties used in the simulation. Boundary conditions were set constant in time and space. A Dirichlet-type thermal boundary condition of 20°C was set at the surface, and an atmospheric cooling rate of 5°C/Km was considered. To reduce the geological uncertainty in the deeper portion of the numerical simulation, the bottom of the model corresponded to that of seismic characterizations in the area (see Hernandez et al., 2020; this volume); 10 Km. However, for testing that the lower boundary condition does not exert a strong control on the result (far-field condition), a model considering a deeper boundary condition, at 20 Km, was also run for comparison; but no major differences were found with the one presented here. Following previous discussions concerning the possible paleo basal heat flow in the sub-Andean ranges of Bolivia (see Rocha and Cristallini, 2015), different values of basal temperature were considered, ranging from 175°C to 300°C. We point out that the examination of several boundary conditions allowed us to compare a group of time-temperature paths modeled in Andino 3D® (each path representing a particular boundary condition), with results from Monte Carlo inversion searching method obtained with HeFTy using the measured (U-Th-Sm)/He data set (Ketcham, 2005; see Hernandez, 2020; this volume). The comparison between HeFTy and Andino 3D® results was made in the Andino3D® environment, as the program also provides tools for this purpose (Fig. 6).

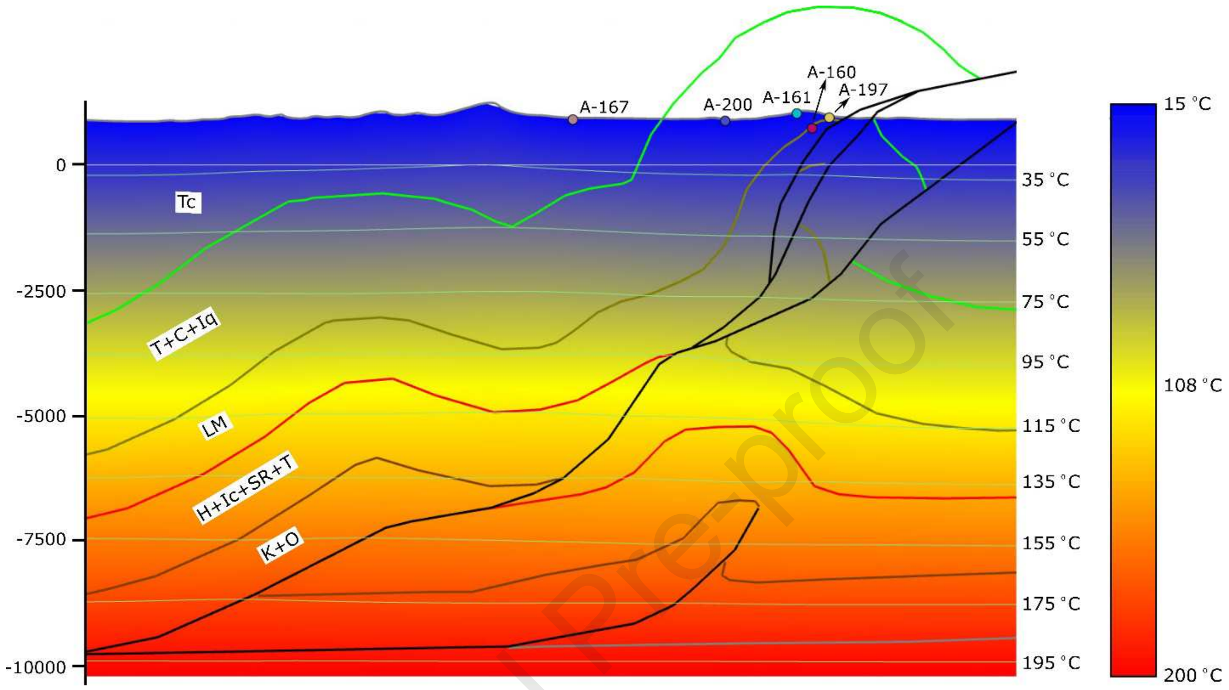


Figure 5: Simplified section used for the Carohuaicho range in Andino 3D®. Yellow lines indicate isotherms. Tc: Tertiary (Cenozoic); T+C+Iq: Tacurú, Carboniferous and Iquiri; LM: Los Monos; H+Ic+SR+T: Huamampampa, Icla, Santa Rosa and Tarabuco; K+O: Kirusillas and Ordovician. The thermal model was run using a constant basal temperature of 200°C, a Dirichlet-type thermal boundary condition of 20° C for the surface, and an atmospheric cooling rate of 5°C/Km.

Table 2 summarizes the results obtained with Andino3D®, as well as those from Hernandez et al., (2020, this volume). We remark the similarity between the values yielded by the Monte Carlo inversion and those from Andino3D®, especially, for the basal temperatures of 200°C and 225°C. Both modeling techniques (inversion of time-temperature paths via Monte Carlo and forward modeling of the heat equation, HeFTy and Andino3D®, respectively) satisfactorily explain the data (see Measured mean age, Table 2). More details about the description and analysis of the thermochronological measurements can be found in Hernandez et al. (2020; this volume).

Sample	Measured	HeFTy	Modeled age for different basal temperatures (Ma)				
	mean age (Ma)	modeled age (Ma)	175 °C	200 °C	225 °C	250 °C	300 °C
A-167	7.2	6.72	7.99	7.78	7.51	7.15	7.2
A-200	3.6	3.73	19.6	7.27	3.61	2.6	1.7
A-161	4.2	3.61	6.91	4.2	3.45	2.79	1.8
A-160	2.7	2.81	2.7	2.7	2.8	2.12	1.37

Table 2: Comparison of mean (U-Th-Sm)/He ages of samples A-167, A-200, A-161 and A-160 with the modeled ages in Andino 3D® for different basal temperatures. Gray columns correspond to the basal temperatures that produce the best fit of age comparison. 200°C is chosen based on this table and the good fitting in time-Temperature charts (see Figure 6). Measured mean ages (Ma) and HeFTy modeled ages (Ma) after Hernandez et al., (2020 in press)

For simplicity, only the results of the numerical simulation considering a basal temperature of 200°C are shown in Fig. 4 and 5. Figure 4 depicts eight balanced structural sections obtained from the kinematic reconstruction and their corresponding thermal state. A brief description of the structural deformation carried out is also given (see Fig. 4). We remark that the display shown in Fig. 4 represents the raw output from the program, shown here to illustrate the integration of thermochronological and structural data in the software. This, likely, represents the first effort that achieves an integrated visualization of the following: a) the structural evolution of a complex structural system, b) the simulated thermal field at each stage of deformation, c) the position (and temperatures) of the samples being modeled, and d) tools for comparison between modeled data and measured data. Since previous forward thermochronological modeling only provided the numerical *solver* to the heat equation and some simplistic structural algorithms (Braun, 2003; Almendral, 2015), it is highlighted that the present work constitutes the first-ever software providing both refined structural capabilities and 2D thermochronological simulations.

Regarding the thermo-kinematic evolution of the Carohuaicho anticline, it can be seen that deformation and uplift were uncorrelated during the first 3 Ma (Fig. 4; see paleo-location of modeled samples). Accommodation of deformation in the system in the period 7 to 4 Ma, resulting in the main structure that crops out today in the Carohuaicho region (see green line depicting the top of Tacurú Formation), caused only minimal vertical displacement of the Devonian-to-Tertiary strata, where the samples considered are located. This effect is related to the deformational process that took place at that time, and that mainly involved the eastward transport of the western limb of the initial anticline of Carohuaicho (modeled with Trishear kinematics; see Erslev, 1991). As the samples are located in the western sector of the anticline, they practically did not undergo uplift during this period (7-4 Ma, see Fig. 4). This observation adds to the discussion on the relationship between slip along a fault and exhumation (and consequent cooling), which, as pointed out previously (see Nassif et al., 2019), might not always be correlated.

From 3 Ma to present, the out-of-sequence thrusting (see details in Hernández et al, 2020) caused most of the vertical denudation of the structure (see Fig. 4, 3 Ma to 0 Ma) and cooling of the samples considered. It is remarked that neither the deformation carried out in the system during the first half of the simulation (Fig. 4; from 7 Ma to 4 Ma), nor the exhumation caused by the out-of-sequence break-through thrusting (Fig. 4; from 3 Ma to present) modified substantially the (initial) thermal configuration of the geological system of Carohuaicho. The final thermal state is depicted in Fig 5, along with samples position and a brief description of the strata composing the anticline (see Table 1 for description of stratigraphic layers). It can be seen that the thermal state today resembles almost a linear equilibrium, implying that the substantial amount of erosion experienced by the system during the last 3 Ma, evidenced by the length of the structural horizons above the mean sea level (see lines depicting tops of stratigraphic layers, Fig. 5, and mean sea level position, 0 Km of altitude), produced no major effect on the underground thermal field of the anticline.

Comparison of results from Andino 3D® with Monte-Carlo inverted time-temperature paths (see Hernandez et al., 2020; this volume), allows one to: a) select the best-fit value for the basal temperature (see Fig. 6) and b) compare results from forward (Andino 3D®) and inverse (HeFTy) numerical procedures. It can be noted that, as expected from their stratigraphic positions, Carboniferous-Devonian samples (A-200, A-161, A-160) exhibit higher temperatures (see Fig. 6) than the Cenozoic sample (A-167).

Moreover, we note that despite the substantial depth (around 3 Km, see Fig. 4, 7 Ma) of some pre-Cenozoic samples before deformation (see A-200, A-161), the maximum temperatures rendered by the inversion procedure (see gray areas in Fig. 6) are barely higher than 80 °C. This is disclosed by both the Monte Carlo inversion as well as by the forward modeling technique (Andino 3D®), since only low geothermal gradients in forward simulations seem to explain the radiometric measurements (see time-temperature paths for each of the basal temperatures considered in Andino 3D®, Fig. 6). Moreover, consistent with previous remarks on exhumation promoted by the out-of-sequence thrusting during the last 3 Ma (see above), it can be noted that all inversion results (all samples) point to a major episode of cooling during the last 3 Myrs, equivalent to the one disclosed by the thermo-kinematic modeling. Again, time-temperature paths from HeFTy for the last 3 Ma of the simulation, are reproduced satisfactorily by simulations from Andino3D® involving basal temperatures below 250°C (i.e, low geothermal gradient, < 30°C/Km). Models with a basal boundary condition of constant heat flow of 45 mWm^2 were tested with very similar results. Altogether, the findings presented not only highlight the feasibility of the kinematic history proposed for the Carohuaicho anticline (see also Hernandez et al., 2020) but also, the validity of the thermochronological simulation developed in Andino 3D.

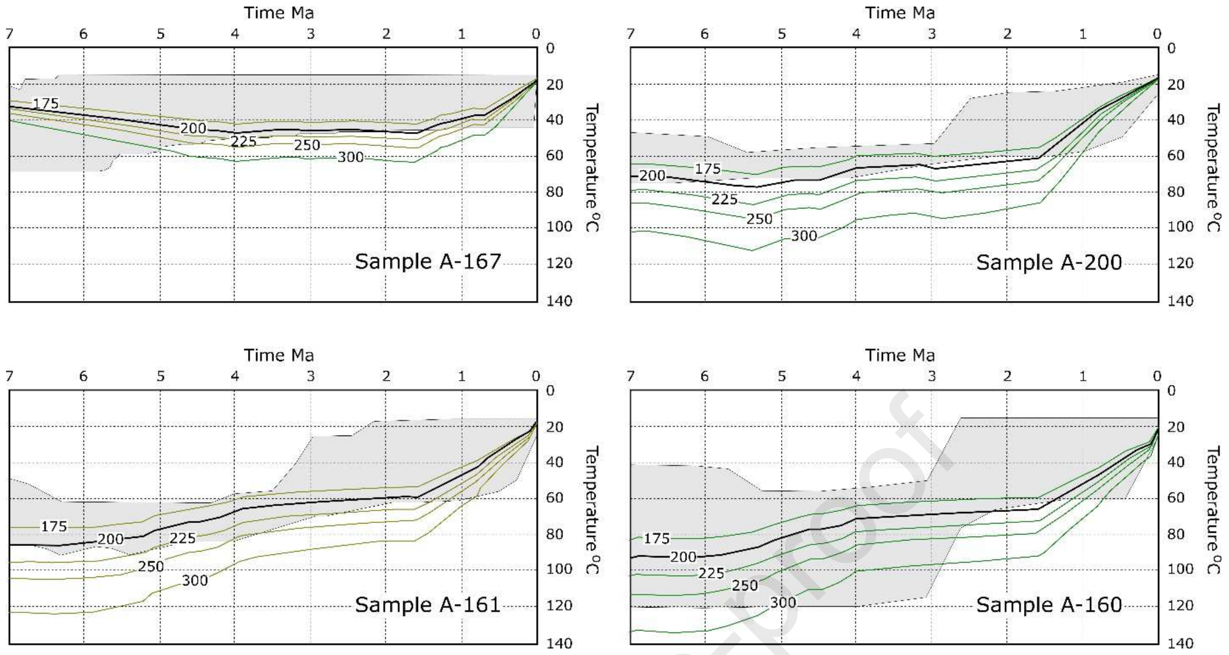


Figure 6: Time-Temperature chart for samples A-167, A-200, A-161 and A160. Different forward models were performed in Andino 3D® with different basal temperatures from 175°C to 300°C to compare with inverse (HeFTy) numerical procedures. Gray zone indicates the envelope of acceptable paths from HeFTy. Bold lines correspond to 200°C model that is the one chosen based on the good fit of these graphics and the modeled ages (see table 2).

Conclusion

The incorporation of Fetkin to Andino 3D® software constitutes the result of joining efforts across different countries and institutions. Previous complex workflows for 2D thermochronological modeling, likely involving the use of several programs, have been consolidated into four steps in the Andino 3D® environment. In addition, the case of study analyzed in this work, the anticline of Carohuaicho in the sub-Andean Ranges of Bolivia, shows the plausibility of the integrated methodology here presented. By granting thermochronologists an easy-to-use tool, we hope this new version of Andino 3D® complements previous modeling efforts (Ketcham, 2005; Gallagher, 2012; Braun, 2003; among others) and facilitates unraveling the thermal histories of geological settings.

Acknowledgement

This work was founded by LA.TE. ANDES S.A. and by CONICET-PDTS.

For further interest in the software, please contact info@lateandes.com or visit the software webpage (www.andino3.com.ar).

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Sample	Inherited age (Ma)	Measured mean age (Ma)	HeFTy modeled age (Ma)	Modeled age for different basal temperatures (Ma)				
				175 °C	200 °C	225 °C	250 °C	300 °C
A-167	8.86	7.2	6.72	7.99	7.78	7.51	7.15	7.2
A-200	300	3.6	3.73	19.6	7.27	3.61	2.6	1.7
A-161	345	4.2	3.61	6.91	4.2	3.45	2.79	1.8
A-197	323	61.6	not modeled	21.8	8.68	5.47	4.41	3
A-160	371	2.7	2.81	2.7	2.7	2.8	2.12	1.37

Units	**Rock types**	**Density** Kg/m^3	**Thermal conductivity W/(m °K)**	**Caloric capacity J/(kg °K)**
Cenozoic units	Sandstones and shales	2760	2.5	865
Tacurú + Carboniferous units + Iquiri	Sandstones and shales	2780	2.6	850
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Huamampampa + Icla + Santa Rosa + Tarabuco	Quarcites, sandstones and shales	2780	2.6	850
Kirusillas + Ordovician	Shales and sandstones	2710	2.3	860

Highlights

- Andino 3D – Fetkin integration provides the user an all-in-one program where thermochronological and structural models can be done.

- Simulated fission track ages, (U-Th-Sm)/He ages and vitrinite %Ro can be simulated for samples positions in Andino 3D.

- Application of Andino 3D thermochronological simulation to Carohuaicho structure in Bolivian Subandean is in agreement with low geothermal gradient, (< 30°C/Km) for the last 7 Ma.

Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: