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Effective closure temperature in leaky and/or saturating thermochronometers

Benny Guralnik[a,b,*], Mayank Jain[b], Frédéric Herman[c], Richard B. Paris[d], T. Mark Harrison[e], Andrew S. Murray[f], Pierre G. Valla[a,c], Edward J. Rhodes[e]

[a] Department of Earth Sciences, ETH-Zurich, 8092 Zurich, Switzerland
[b] Centre for Nuclear Technologies, Technical University of Denmark, DTU Risø Campus, DK 4000 Roskilde, Denmark
[c] Faculty of Geosciences and Environment, University of Lausanne, CH-1015 Lausanne, Switzerland
[d] University of Abertay, Dundee DD1 1HG, UK
[e] Department of Earth and Space Sciences, UCLA, Los Angeles, CA 90095-1567, USA
[f] Nordic Laboratory for Luminescence Dating, Department of Geoscience, Aarhus University, DTU Risø Campus, Denmark

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ABSTRACT

The classical equation of closure temperature (T_C) in thermochronometry (Dodson, 1973), assumed (i) no storage limitation for the accumulating radiogenic product, (ii) a negligible product concentration at the initial temperature of cooling T_0, and (iii) a negligible product loss at the final (present-day) temperature T_P. A subsequent extension (Ganguly and Tirone, 1999) provided a simple correction for systems cooling from an arbitrary T_0, at which presence of an initial concentration profile may affect final concentrations. Here, we use a combination of analytical and numerical solutions to derive a general expression for the effective closure temperature in (i) systems which cool between arbitrary initial and final temperatures, potentially still suffering from thermal product loss at T_P (termed 'leaky'), and (ii) systems which may contain a physical limit on the maximum amount of product that can be stored (termed 'saturating'). While all conservative results can be easily reproduced, an extended use of our formulation provides meaningful effective closure temperatures even when the standard calculation schemes fail. For a first-order loss radiometric system governed by $K(T) = s\exp(-E/RT)$, where E [$\mathrm{J\,mol^{-1}}$] and s [$\mathrm{s^{-1}}$] are the Arrhenius parameters and R is the gas constant, we find that the effective closure temperature $T_C(T_0, T_P)$ is given by:

$$T_C(T_0,T_P)=\left\{\frac{1}{T_P}-\frac{R/E}{\tau\lambda-\tau K_P}\ln\left[1+\frac{\tau\lambda-\tau K_P}{(\tau K_P)^{\tau\lambda}e^{-\tau K_P}}\bigl(\Gamma(\tau\lambda,\tau K_P)-\Gamma(\tau\lambda,\tau K_0)\bigr)\right]\right\}^{-1}$$

where K_0 and K_P [$\mathrm{s^{-1}}$] are shorthand for $K(T_0)$ and $K(T_P)$, respectively, λ [$\mathrm{s^{-1}}$] the production rate, τ [s] a time constant, and $\Gamma(a, z)$ the upper incomplete gamma function. Under conventional conditions, our solution reduces to Dodson's formula. Although the solution strictly applies only to systems where $1/T$ increases linearly with time, it is nevertheless a useful approximation for a broad range of cooling functions in systems where closure occurs close to the system's initial/final thermal boundary conditions. We clarify the use and the meaning of $T_C(T_0, T_P)$ by drawing a comparison between (i) a hypothetical application of apatite U–Pb dating ($T_C \approx 450\,^\circ$C) on Venus (mean surface temperature of $450\,^\circ$C, leaky behaviour), and (ii) the recently introduced thermochronometric application of optically stimulated luminescence (OSL) dating on Earth (both leaky and saturating behaviour).

1. Introduction

Thermochronometry is based on the observation that transport of radiogenic/fissionogenic products within their host crystals is temperature-dependent. Consequently, a crystal may behave as an 'open' or a 'closed' system to a certain product, depending on the rate of its thermal diffusion/annealing. In noble gas thermochronometers (Harrison and Zeitler, 2005), the frequency K [$\mathrm{s^{-1}}$] at which radiogenic atoms get thermally mobilised and removed from their production sites tends to follow an Arrhenius law:

$$K(T) = s\exp(-E/RT) \tag{1}$$

* Corresponding author at: Department of Earth Sciences, ETH-Zurich, 8092 Zurich, Switzerland.
E-mail address: benny.guralnik@gmail.com (B. Guralnik).

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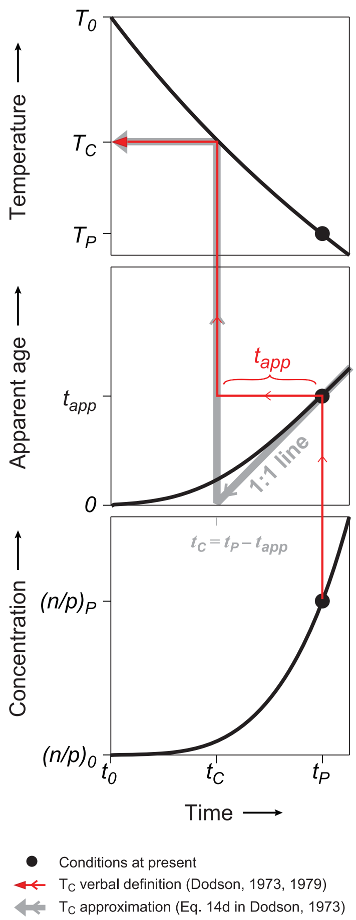

Fig. 1. Evolution of temperature (top panel), radiogenic product concentration (bottom panel), and the apparent age (central panel) in a thermochronometric system cooling from an arbitrary time in the past (t_0) until the present-day (t_P; thick circles on panels mark present-day conditions). By definition, Dodson's effective closure temperature can be graphically found (thin red arrowed line on all panels; Eq. (6)) by converting present-day product/parent ratio $(n/p)_P$ (bottom panel) into an apparent age t_{app} (central panel), rolling back an equivalent amount of time to find the closure time t_C (central panel), and reading off the corresponding palaeotemperature T_C (red arrowhead on top panel). In Dodson's standard approximation (thick grey arrowed line on central and top panels; Eq. (3)) the initial step of converting concentration into age is omitted, and the closure time t_C is found directly by intersecting the linear asymptote to apparent age (1:1 line) with the time axis (central panel). For the thermal scenario shown, both calculation schemes (Eqs. (6) and (3), respectively) yield an identical result (overlapping red and grey arrowheads on top panel, respectively). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

where s [s^{-1}] is the frequency factor, E [J mol^{-1}] the activation energy, R the gas constant, and T [K] the ambient temperature (Langmuir, 1923; Philibert, 2006). The linear proportionality between $\log(K)$ and T^{-1}, determined by diffusion and annealing experiments in the laboratory, yields the kinetic parameters E and s which can then be extrapolated across a wide range of temperatures and geological timescales.

The recognition that any radiometric age represents the time at which the corresponding system cooled below an effective thermal threshold to enable product accumulation, led to the abstract concept of 'closure temperature' T_C (Dodson, 1973) and promoted the widespread use of thermochronometry in earth sciences. Dodson defined T_C as 'the temperature of the system at the time represented by its apparent age' (Dodson, 1973, 1979). Fig. 1 tracks a thermochronometer through the evolution of its temperature (top panel), concentration (bottom panel), and the apparent age (central panel) through time. Closure temperature T_C can be graphically found using either (i) Dodson's precise wording or (ii) Dodson's classical approximation. Note that the verbatim definition of T_C (thin red arrowed line; Eq. (6)) involves measuring the daughter/parent ratio $(n/p)_P$ at the present-day time t_P (circle on lower panel), converting this concentration into an apparent age t_{app} (circle on central panel) to obtain the time of closure $t_C = t_P - t_{app}$, and finally reading off the corresponding palaeotemperature T_C (red arrowhead on top panel); Dodson's widely-used approximation (thick grey arrowed line; Eq. (3)) skips the first step of age determination, but typically yields identical results.

Noting that T_C must depend on the precise cooling history, Dodson (1973) adopted a benchmark thermal scenario in which $1/T$ increases linearly with time:

$$E/RT = E/RT_0 + t/\tau \tag{2}$$

where T_0 [K] is the initial temperature, t [s] the time and τ [s] the 'time constant' (Dodson, 1973). The latter, frequently called 'characteristic time' (e.g. Ganguly and Tirone, 1999), corresponds to the time taken for E/RT to increase by 1, or for K to diminish by a factor e^{-1} (through substitution of Eq. (2) into Eq. (1)). This hyperbolic relationship of $1/T \propto t$ turned out to be particularly useful, since it allowed approximation of both exponentially-decaying and semi-linear cooling scenarios (e.g. Newton's cooling law vs. rapid exhumation) through a simple adjustment of τ, T_0 and T_P. Equipped with such prescribed cooling history, Dodson proceeded to solve the governing rate equation (Eq. (A.1) in Appendix A) to obtain a general approximation for T_C:

$$E/RT_C = \ln\left(\tau s \gamma^{-1}\right), \quad \gamma = \left[\Gamma(\lambda\tau + 1)\right]^{1/\lambda\tau} \tag{3}$$

(Dodson, 1973, Eq. (14d)) where $\Gamma(z)$ is the Gamma function (Abramowitz and Stegun, 1964). The essence of Dodson's approximation is visualised by the thick grey arrowed line in Fig. 1, clarifying one frequently overlooked fact: while n/p may evolve in an absolutely non-linear manner (e.g., in the general case of a short-lived parent), it is strictly the apparent age t_{app} (Fig. 1, black curve on central panel) which at large times asymptotes to a line with a slope of 1 (meaning that the concentration-derived apparent age paces in synchrony with time, i.e. $dt_{app}/dt \to 1$). Calculation of T_C using Eq. (3) simply amounts to finding the linear asymptote to the apparent age function at large times (Fig. 1, 1:1 line on central panel), intersecting it with the time axis to get t_C, and reading off the corresponding palaeotemperature T_C (Fig. 1, grey arrowhead on top panel). For the typical thermal scenario depicted on Fig. 1, both the verbatim and the approximated calculation schemes (thin red and thick grey arrowed lines, respectively) yield indistinguishable values of T_C.

The classical way to reconstruct thermal histories via the closure temperature concept is to measure a set of (t_{app}, T_C) values using multiple thermochronometric systems, each providing a marker on the time–temperature space (Wagner et al., 1977). Note, that unlike the apparent age t_{app}, which exhibits a power-law relationship with τ (Eq. (A.7)), the closure temperature T_c does only weakly depend on τ (Dodson, 1973). For end-user convenience, τ has been typically replaced with $\tau = RT_C^2/E\dot{T}$ (Dodson, 1973), where $\dot{T} = -dT/dt$ is the linear cooling rate in the vicinity of closure, and a much more 'intuitive' quantity than τ. The dependence of T_C on $\dot{T}$ can be exploited to approximate the cooling history of known-age rocks (Ganguly and Tirone, 2009), and used as a baseline for methodological comparison between different thermochronometers (e.g. Reiners and Brandon, 2006).

An increasing interest in low-temperature proxies capable of recording the very last stages of rock cooling (e.g., Reiners and Ehlers, 2005) has been typified by the development of thermochronometers based on ^{4}He/^{3}He profiling (Shuster and Farley, 2005) and optically stimulated luminescence (OSL) dating (Herman et al., 2010). Although Dodson's T_C concept may at first seem to