PROGRAMS FOR ILLUSTRATING CLOSURE, PARTIAL RETENTION, AND THE RESPONSE OF COOLING AGES TO EROSION: CLOSURE, AGE2EDOT, AND RESPTIME

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Overview

CLOSURE, AGE2EDOT, and RESPTIME are a set of simple programs that were first developed in Brandon et al. (1998). They were designed to help demonstrate the influence of steady and transient erosion on fission-track (FT) cooling ages. The programs have since been extended to include (U-Th)/He and $^{40}Ar/^{39}Ar$ ages, as well as FT ages. The programs now include modern diffusion data for all of the minerals commonly dated for thermochronometry, ranging from He dating of apatite to Ar dating of hornblende.

CLOSURE is a standard Windows-style program, whereas AGE2EDOT and RESPTIME are console-style programs. All of the programs are compiled for the Windows operating system. Each consists of a single exe file. Setup involves copying the file into a suitable directory. The programs are started by double-clicking the file name. The programs require no input files. Rather, the user is guided by a set of prompts and questions to supply the necessary input parameters for the calculation of interest. Results are output to a window for CLOSURE and to an output file for AGE2EDOT and RESPTIME. In all cases, the output is organized with tab-separated columns, so that it can be easily imported into a plotting program, such as EXCEL or SIGMAPLOT.

Upgrades will be posted at www.geology.yale.edu/~brandon. The source code for the programs is available on request.

Methods for CLOSURE

The CLOSURE program provides a compilation of the data needed to calculate effective closure temperatures and partial retention temperatures for all of the minerals commonly dated by the He, FT, and Ar methods (Figure 1). Laboratory diffusion experiments have demonstrated that, on laboratory time scales, the diffusivity of He and Ar are well fit by

$$D = D_0 \exp\left[\frac{-E_a - PV_a}{RT}\right], \qquad (1)//$$

where D_0 is the frequency factor (m^2 s^{-1}), E_a is the activation energy (J mol^{-1}), P is pressure (Pa), V_a is the activation volume (m^3 mol^{-1}), T is temperature (K), R is the gas law constant (8.3145 J mol^{-1} K^{-1}), and D is the diffusivity (m^2 s^{-1}). The $P\ V_a$ term is commonly set to zero, since its contribution is generally small relative to E_a. D_0 and E_a are compiled in Tables 1 and 2 for the main minerals dated by the He and Ar method.

The *partial retention zone* is defined in two ways. This concept was first introduced to account for partial annealing of fission tracks when held at a steady temperature. Laboratory heating experiments were used to define the time-temperature conditions that caused 90% and 10% retention of the initial density of fossil tracks. The retention behavior was considered for loss only, without regard for the production of new tracks during the heating event. We use the term loss-only PRZ to refer to this kind of partial retention zone for He, FT, and Ar dating. Figures 2-4 show examples of loss-only PRZs. They help to illustrate the time and temperature conditions needed to fully preserve or fully reset a He, FT, or Ar cooling age.

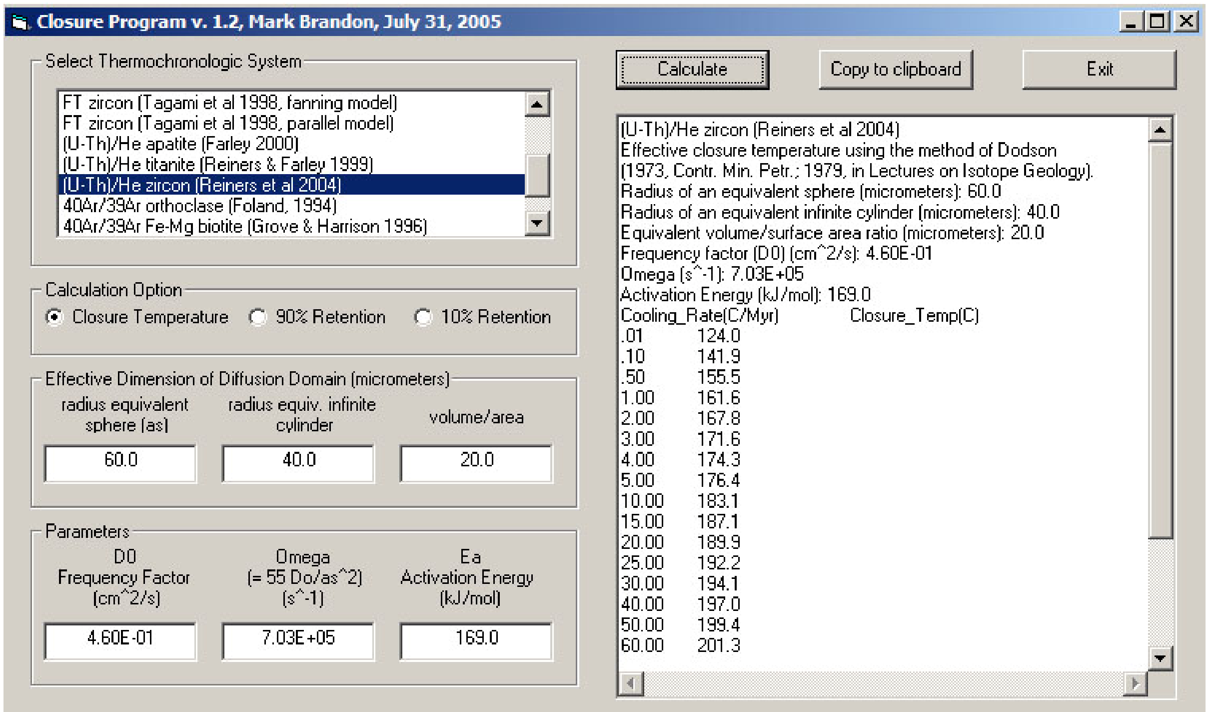

Figure 1. Screen image of the CLOSURE program showing a typical run result.

Table 1. Closure parameters for He and FT dating.

Method (references)	E_a (kJ mol^{-1})	D_0 (cm^2 s^{-1})	a_s [4] (μm)	Ω [5] (s^{-1})	$T_{c,10}$ [6] (C)
(U-Th)/He apatite (Farley, 2000)	138	50	60	7.64×10^7	67
(U-Th)/He zircon (Reiners et al., 2004)	169	0.46	60	7.03×10^5	183
(U-Th)/He titanite (Reiners and Farley, 1999)	187	60	150	1.47×10^7	200
FT apatite[1] (average composition[2]) (Ketcham et al., 1999)	147	--	--	2.05×10^6	116
FT Renfrew apatite[3] (low retentivity) (Ketcham et al., 1999)	138	--	--	5.08×10^5	104
FT Tioga apatite[3] (high retentivity) (Ketcham et al., 1999)	187	--	--	1.57×10^8	177
FT apatite (Durango) (Laslett et al., 1987; Green, 1988)	187	--	--	9.83×10^{11}	113
FT zircon[1] (natural, radiation damaged) (Brandon et al, 1998)	208	--	--	1.00×10^8	232
FT zircon (no radiation damaged) (Rahn et al., 2004, fanning model)	321	--	--	5.66×10^{13}	342
FT zircon (Tagami et al., 1998, fanning model)	324	--	--	1.64×10^{14}	338
FT zircon (Tagami et al., 1998, parallel model)	297	--	--	2.56×10^{12}	326

Footnotes;

1) Recommended values for most geologic applications.

2) Average composition was taken from Table 4 in Carlson et al. (1999). Equation 6 in Carlson et al. (1999) was used to estimate r_{mr0} = 0.810 for this composition. Closure parameters were then estimated using the HeFTy program (Ketcham, 2005).

3) Closure parameters were estimated from HeFTy and r_{mr0} = 0.8464 and 0.1398 for Renfrew and Tioga apatites, respectively, as reported in Ketcham et al. (1999).

4) a_s is the effective spherical radius for the diffusion domain. Shown here are typical values.

5) Ω is measured directly for FT thermochronometers, and is equal to $55D_0a_s^{-2}$ for He and Ar thermochronometers.

6) $T_{c,10}$ is the effective closure temperature for 10 C Ma^{-1} cooling rate and specified a_s value.

Table 2. Closure parameters for Ar dating.

Method (references)	E_a (kJ mol^{-1})	D_0 (cm^2 s^{-1})	a_s [1] (μm)	Ω [2] (s^{-1})	$T_{c,10}$ [3] (C)
$^{40}Ar/^{39}Ar$ K-feldspar (orthoclase) Foland (1994)	183	9.80 x 10^{-3}	10	5.39 x 10^5	223
$^{40}Ar/^{39}Ar$ Fe-Mg biotite Grove and Harrison (1996)	197	7.50 x 10^{-2}	750 (500)	733	348
$^{40}Ar/^{39}Ar$ muscovite Robbins, 1972; Hamres and Bowring, 1994)	180	4.00 x 10^{-4}	750 (500)	3.91	380
$^{40}Ar/^{39}Ar$ hornblende Harrison (1981)	268	6.00 x 10^{-2}	500	1320	553

Footnotes:

1) a_s is the effective spherical radius for the diffusion domain. Shown here are typical values. Muscovite and biotite have cylindrical diffusion domains, with typical cylindrical radii shown in parentheses. For these cases, a_s is approximated by multiplying the cylindrical radius by 1.5.

2) Ω is equal to $55 D_0 a_s^{-2}$ for Ar thermochronometers.

3) $T_{c,10}$ is the effective closure temperature for 10 C Ma^{-1} cooling rate and specified a_s value.

Table 3. Parameters for FT partial retention zones.

Method (references)	Retention Level	E_a (kJ mol^{-1})	Ω [4] (s^{-1})
FT apatite[1] (average composition[2]) (Ketcham et al., 1999)	90%	127	2.67×10^{5}
	10%	161	1.55×10^{7}
FT Renfrew apatite[3] (low retentivity) (Ketcham et al., 1999)	90%	124	1.91×10^{5}
	10%	150	4.39×10^{6}
FT Tioga apatite[3] (high retentivity) (Ketcham et al., 1999)	90%	140	1.41×10^{6}
	10%	232	3.38×10^{10}
FT Durango apatite (Laslett et al., 1987; Green, 1988)	90%	160	1.02×10^{12}
	10%	195	2.07×10^{12}
FT zircon[1] (natural, radiation damaged) (Brandon et al, 1998)	90%	225	2.62×10^{11}
	10%	221	1.24×10^{8}
FT zircon (no radiation damage) (Rahn et al., 2004, fanning model)	90%	272	5.66×10^{13}
	10%	339	5.66×10^{13}
FT zircon (Tagami et al., 1998, fanning model)	90%	231	1.09×10^{12}
	10%	359	1.02×10^{15}
FT zircon (Tagami et al., 1998, parallel model)	90%	297	5.94×10^{15}
	10%	297	1.51×10^{11}

Footnotes:

1) Recommended values for most geologic applications.

2) Average composition was taken from Table 4 in Carlson et al. (1999). Equation 6 in Carlson et al. (1999) was used to estimate $r_{mr0} = 0.810$ for this composition. PRZ parameters were then estimated using the HeFTy program (Ketcham, 2005).

3) PRZ parameters were estimated from HeFTy and $r_{mr0} = 0.8464$ and 0.1398 for Renfrew and Tioga apatites, respectively, as reported in Ketcham et al. (1999).

4) Ω is measured directly for FT thermochronometers

The loss-only PRZ is calculated for He and Ar dating using the exact version of the loss-only diffusion equation (spherical geometry) from McDougall and Harrison (1999). The equations require D_0 and E_a as parameters, as given in Tables 1 and 2.

Wolf and Farley (1998) defined a different kind of PRZ, one that accounted for both production and loss of the ^4He, FT, or ^{40}Ar. The limits of the loss-and-production PRZ are defined by the temperatures needed to maintain a He, FT, or Ar age that is 90% or 10% of the hold time. The time-temperature conditions associated with this 90% and 10% retention are determined using the loss-and-production equations in Wolf and Farley (1998). The equations require D_0 and E_a as parameters. This kind of PRZ is useful for considering how the measured age for a thermochronometer will change down a borehole, as a function of downward increasing but otherwise steady temperatures.

The CLOSURE program estimates both types of PRZ for He and Ar methods. It only calculates the loss-only PRZ for FT methods. Annealing models, such as HeFTy (Ketcham, 2005) could be used to calculate a loss-and-production PRZ for the FT apatite system, but there is no such model yet for annealing and production for the FT zircon system. The 90% and 10% retention isopleths are determined from time-temperature results from laboratory stepwise-heating experiments. The isopleths commonly have an exponential form,

$$t = \Omega^{-1} \exp\left[-\frac{E_a}{RT}\right] \tag{2}$$

where *Ea* is the activation energy, **Ω** is the normalized frequency factor, *R* is the gas law constant, *T* is the steady temperature (K), and *t* is the hold time (s). This can be recast into the typical Arrhenius relation,

$$\ln[t] = -\ln[\Omega] - \frac{E_a}{RT}\,. \tag{3}$$

This approach was used to determine *Ea* and **Ω** for 90% and 10% retention minerals dated by the fission track method (Table 3).

Dodson (1973; 1979) showed that for a steady rate of cooling, one could identify an *effective closure temperature* T_c, which corresponds to the temperature at the time indicated by the cool age measured for the thermochronometer. We emphasize that T_c is only defined for the case of steady cooling through the PRZ, but this assumption is reasonable for many eroding mountain belts, given the narrow temperature range for the PRZ and the slow response of the thermal field to external changes. In contrast, this assumption will likely fail for areas affected by local igneous intrusions, hydrothermal circulation, or depositional burial.

Dodson (1973; 1979) estimated T_c using

$$\dot{T}(T_c) = \frac{-\Omega R T_c^2}{E_a} \exp\left[-\frac{E_a}{RT_c}\right], \tag{4}$$

where $\dot{T}(T_c) = \left(\frac{\partial T}{\partial t}\right)_{T=T_c}$ ($\dot{T} < 0$ for cooling), *R* is the gas law constant, and the normalized frequency factor **Ω** and activation energy E_a are closure parameters, as defined in Tables

1 and 2. The cooling rate at T_c is given by $\dot{T} = \left(\frac{\partial T}{\partial z}\right)_{Tc} \dot{\varepsilon}(\tau_c)$, where $\left(\frac{\partial T}{\partial z}\right)_{Tc}$ is the thermal gradient at the closure isotherm, and $\dot{\varepsilon}(\tau_c)$ is the erosion rate at τ_c, the time of closure.

For He and Ar dating, $\Omega = \frac{55D_0}{a_s}$, where a_s is the equivalent spherical radius for the diffusion domain. Tables 1 and 2 list typical values for a_s, but the user will need to judge if a more suitable value is appropriate given the specifics about what has been dated. Most of the minerals dated by He and Ar have isotropic diffusion properties, meaning that He and Ar diffuse at equal rates in all directions (muscovite and biotite are exceptions that are discussed below). Furthermore, the diffusion domains are commonly at the scale of the full mineral grain. The dated minerals may have anisotropic shapes. As an example, zircons and apatites tend to occur as elongate prisms. We can calculate an approximate equivalent spherical radius using

$$a_s \approx 3\frac{V}{A}, \qquad (3)$$

(Fechtig and Kalbitzer, 1966; Meesters and Dunai, 2002), where V and A refer to the volume and surface area of the mineral grain.

Biotite and muscovite are anisotropic, with the fast direction of diffusion parallel to the basal plane, indicating cylindrical diffusion geometry. Equations are available to solve for cylindrical diffusion, but we have opted to approximate the solution by converting the cylindrical radius a_c of the mica grains into an equivalent spherical radius, where $a_s = 1.5\ a_c$, and then using this radius with the spherical solution for the diffusion equations. These approximate scaling relationships are shown for the values under the label “Effective Dimensions of Diffusion Domain (micrometers)”. These approximations are very good for calculating 90% retention and effective closure temperatures. They work less well for calculating the time-temperature conditions for 10% retention.

The Dodson equation can also be applied to the fission-track system (Dodson, 1979). He recommended using Ea and **Ω** determined from the 50% retention isopleth from time-temperature heating experiments. Fission tracks contain a range of defects, created by the flight of the two energetic fragments created by the fission decay reaction of ^{238}U. This situation accounts for why the annealing process has a range of E_a values, which increase with increasing annealing of initial tracks. This observation is thought to mean that there is a range of activation energies needed to drive the diffusion involved in repairing this lattice damage (e.g., Ketcham et al., 1999). We do not know the size of the diffusion domain, which means that we cannot measure D_0. Nonetheless, we can measure **Ω**, which is all that is needed to use the Dodson closure equation. Dodson (1979) argued that the 50% retention isopleth provides the best average values for E_a and **Ω**, given that the cooling path for closure requires moving through the PRZ.

We have estimated these parameters from a range of FT annealing experiments (Tables 2 and 4). We have compared the T_c values calculated with the Dodson equation with those estimated by more complex FT models, such HeFTy. In general, the Dodson estimates for T_c are within ~1 C relative to those given by numerical models.

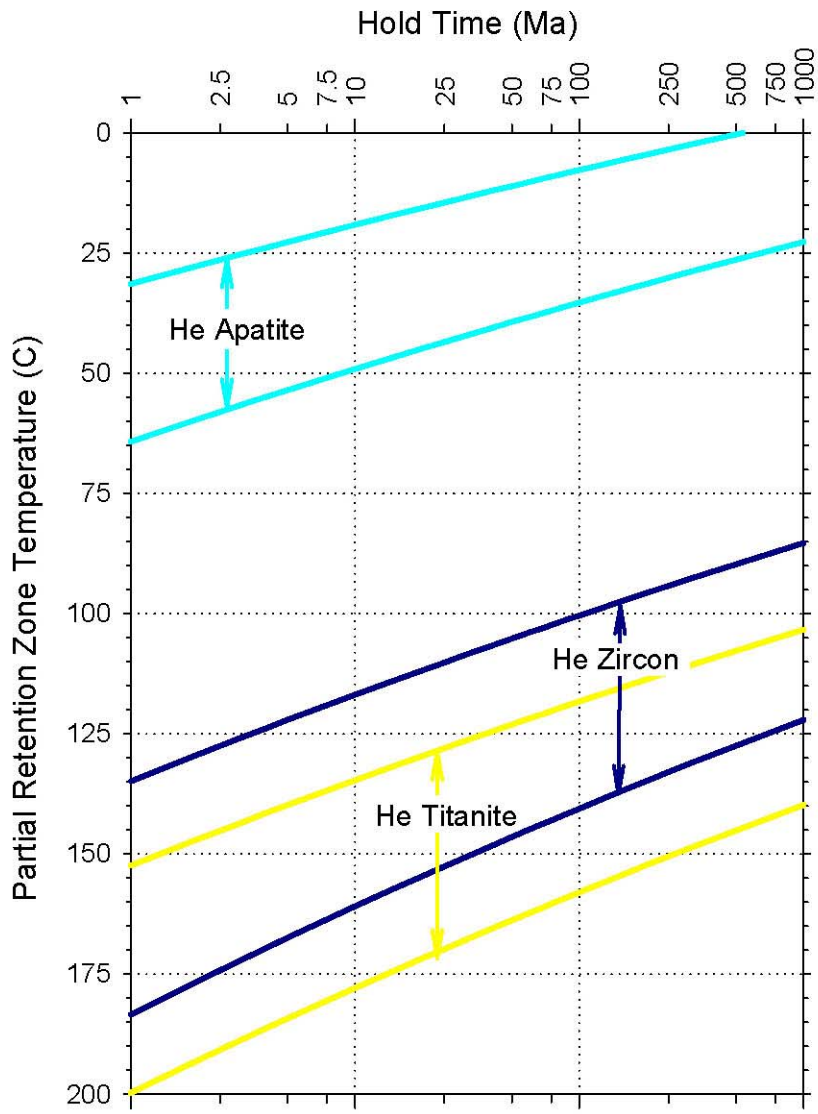

Figure 2. Loss-only PRZ for He dating methods calculated using CLOSURE.

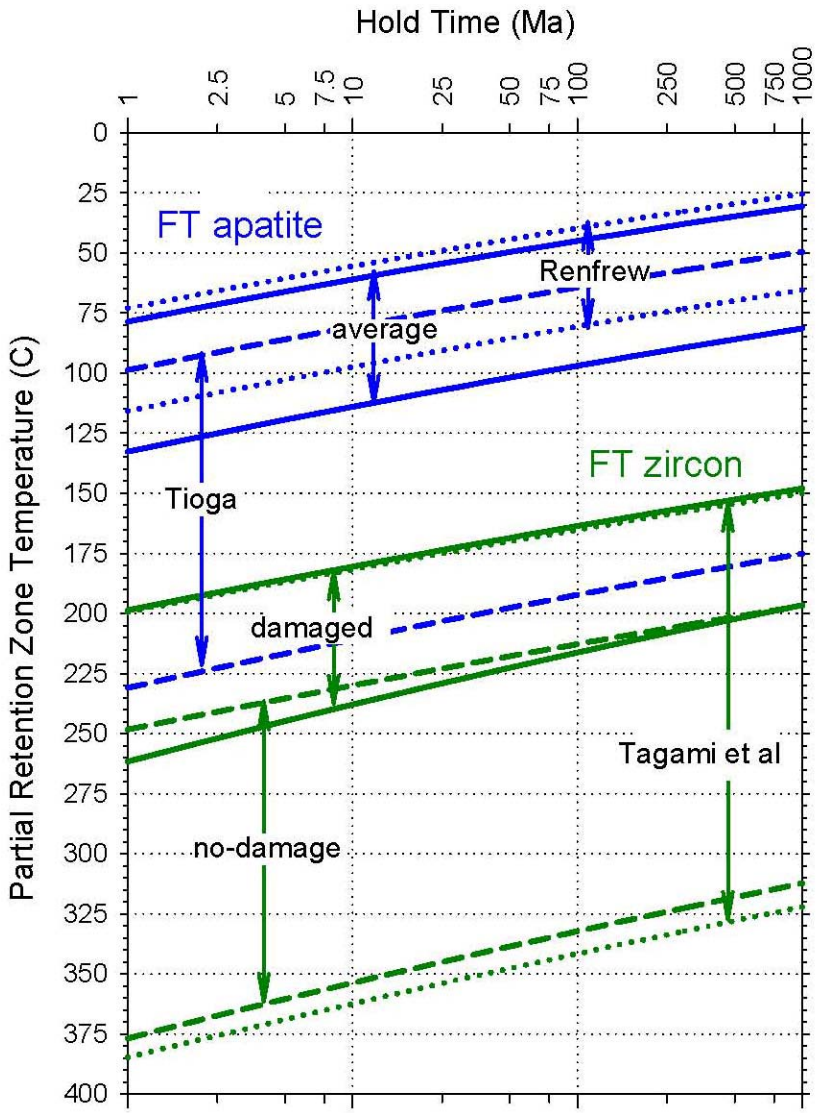

Figure 3. Loss-only PRZ for FT dating calculated using CLOSURE..

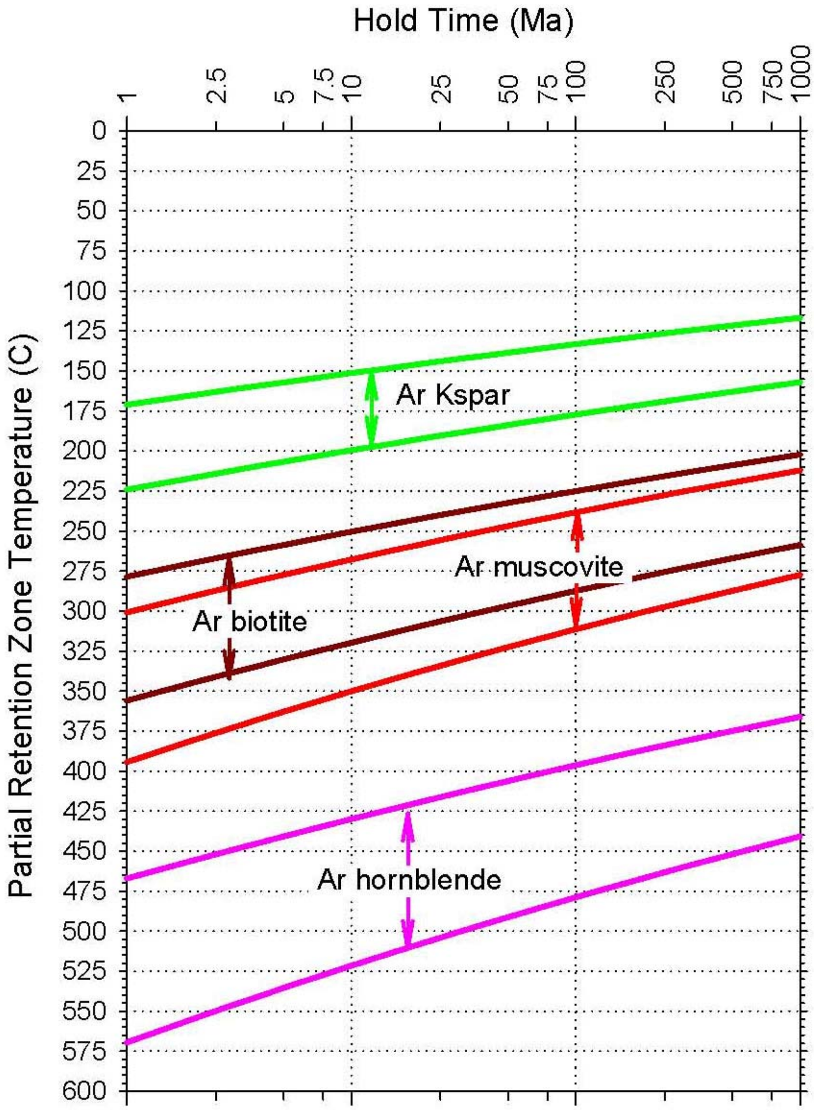

Figure 4. Loss-only PRZ for Ar dating calculated using CLOSURE..

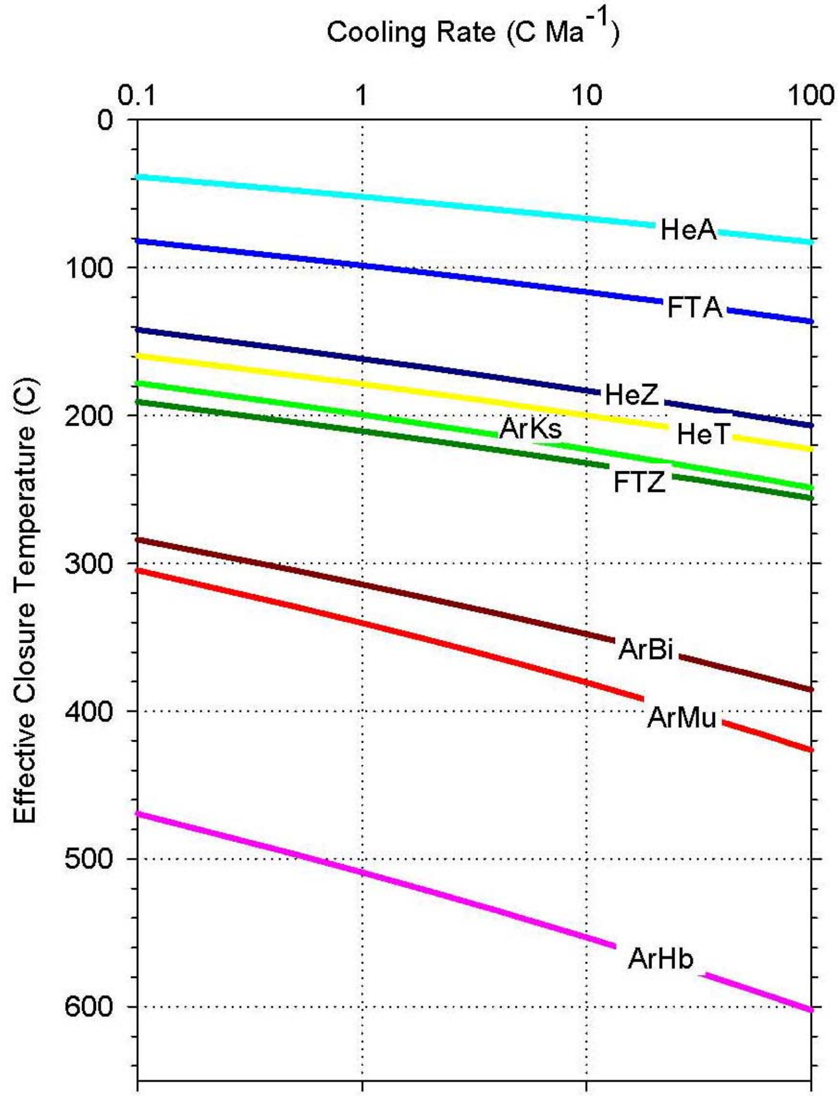

Figure 5. Effective closure temperatures calculated using CLOSURE.

Methods for AGE2EDOT

AGE2EDOT estimates the cooling age for a thermochronometer that was exhumed by steady erosion at a constant rate (Figure 5). The thermal field is represented by the steady-state solution for an infinite layer with a thickness L (km), a thermal diffusivity κ (km^2 Ma^{-1}), a uniform internal heat production H_T, a steady surface temperature T_s and an estimate of the near-surface thermal gradient for no erosion. These thermal parameters are usually estimated, at least in part, from heat flow studies. We use, as an example, thermal parameters for the active convergent orogen in the northern Apennines of Italy, where $L \sim 30$ km, $\kappa \sim 27.4$ km^2 Ma^{-1}, $H_T \sim 4.5$ C Ma^{-1}, $T_s \sim 14$ C, and the zero-erosion surface thermal gradient would be ~20 C km^{-1}. The calculated basal temperature is 540 C, which is held constant throughout the calculation. Material moves through the layer at a constant velocity u. One can envision that this situation simulates a steady-state orogen where underplating is occurring at the same rate as erosion, with $u = \dot{\varepsilon}$. The thickness of the orogen remains steady and the vertical velocity through the wedge would be approximately uniform and steady.

The thermal model provides a full description of the temperature and thermal gradient as a function of depth. The cooling rate is $\dot{T}(T_c) = \left(\frac{\partial T}{\partial z}\right)_{Tc} \dot{\varepsilon}$. Given the cooling rate and the temperature with respective to depth, we can use the Dodson equation to solve for T_c, and for the depth of closure z_c. The predicted cooling age is given by $\frac{z_c}{\dot{\varepsilon}}$.

AGE2EDOT gives a full prediction of how the cooling age for the specified thermochronometer will change as a function of erosion rate. Faster erosion causes isotherms, including the closure isotherm, to migrate closer to the surface. The steeper thermal gradient causes a faster rate of cooling and thus a greater T. The net effect is that the closure depth becomes shallower with faster erosion, but this effect is reduced by the response of the increase in Tc caused by faster cooling.

Brandon et al. (1998) provides more details about this calculation. I provide a example here of the relationship between erosion rate and cooling ages for all of the major thermochronometers. The thermal parameters used are those discussed above for the northern Apennines. An example of the input data and results is given in the file: AGE2EDOT.output.

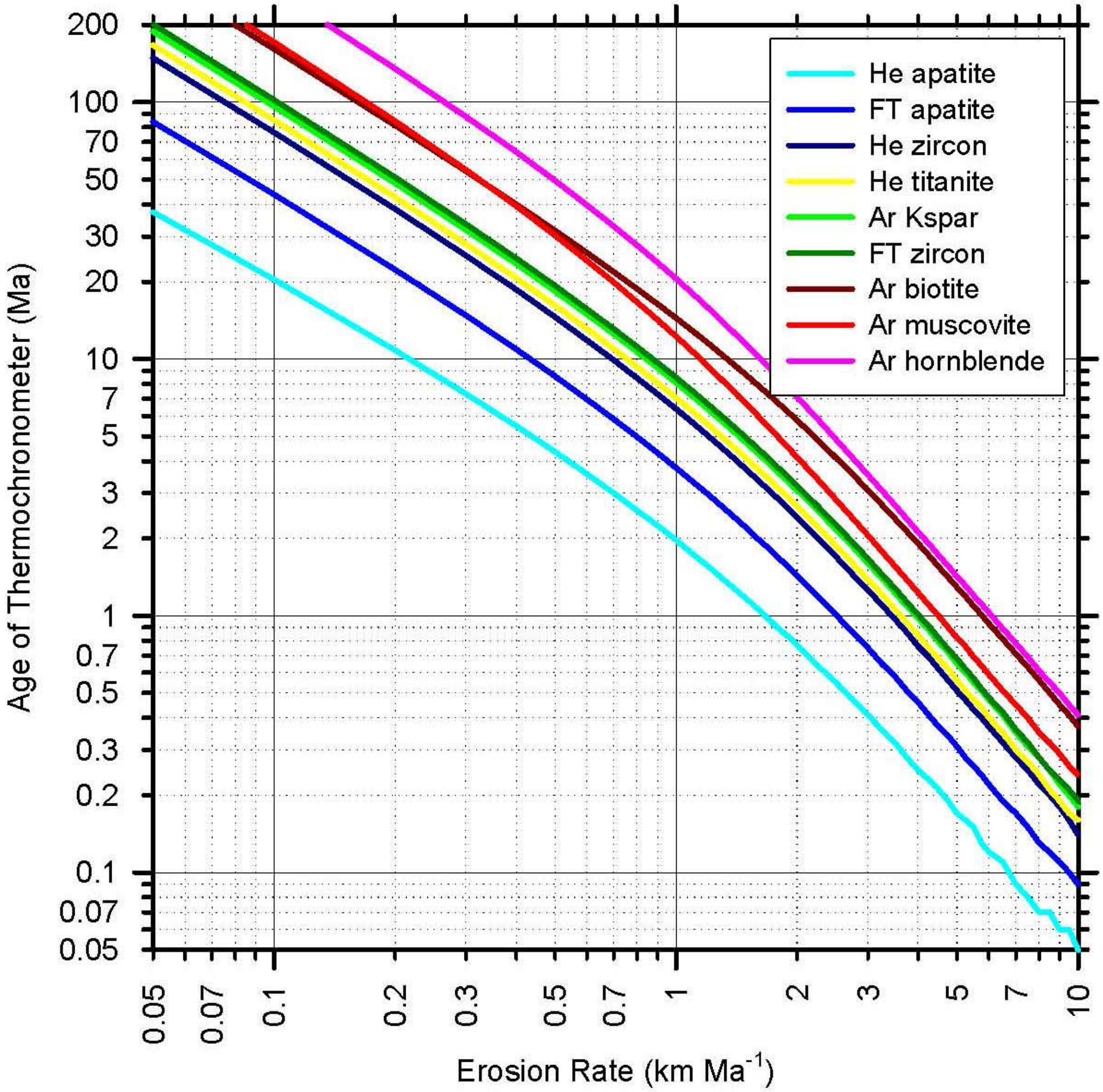

Figure 6. Age versus erosion rate for all of the major thermochronometers. Calculated using AGE2EDOT.

Methods for RESPTIME

RESPTIME calculates the migration of the closure isotherm due to an instantaneous change in erosion rate. The program is similar to AGE2EDOT but it uses a finite-difference algorithm to solve for the evolution of 1D thermal field in an infinite layer. Figure 7 shows plots of the response of all of the major thermochronometers to a instantaneous change from no erosion before 0 Ma to steady erosion at a rate of 1 km Ma^{-1}. Thermal parameters used are identical to the northern Apennines values used for the example for AGE2EDOT. The distribution package includes a sample output file from this example (see the file called RESPTME.output). Note that L was increased to 50 km for the Ar muscovite and Ar hornblende calculations, in order to ensure that T_c remained within the layer for these high-temperature thermochronometers.

The motion of the closure isotherm is represented in Figure 7 by its normalized velocity, which is defined by the vertical velocity of the isotherm divided by the erosion rate. A normalized velocity of zero means that the closure isotherm has reached a steady-state position; whereas a normalized velocity of one means that the isotherm is moving upward at the same rate as the rock. There would be no cooling at this stage.

Figure 7 shows that the normalized velocity for the closure isotherm for the He thermochronometer slows down to <10% within 2.5 Ma following the start of fast erosion. In contrast, it takes 16 Ma for the Ar muscovite system to reach the 10% level. This example highlights the importance for using low-temperature thermochronometers for measuring erosion rates.

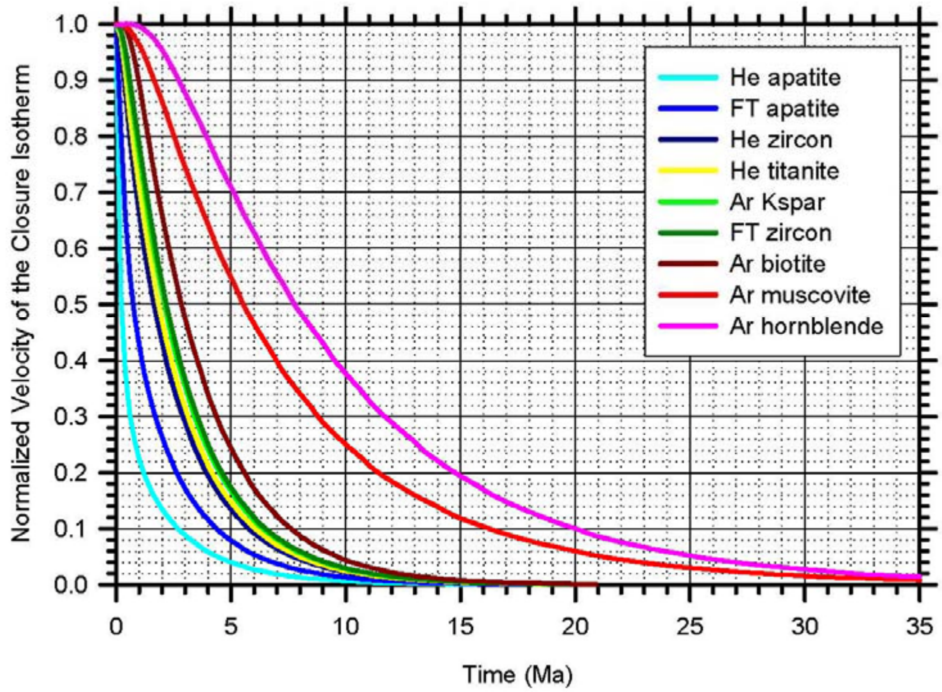

Figure 7. Response time of closure isotherms for the listed thermochrometers due to an instantaneous increase in erosion rate at time 0 Ma, from no erosion to 1 km Ma^{-1}. Calculated using RESPTIME.

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