Closure Temperature

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Outline

1. Physical background;
2. Transformation of time variable;
3. Atomistic interpretation of “closing”, “freezing”;

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Some definitions

Layman asks: What is closing temperature???

Expert answers: Closing temperature is an individual concept !!!

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Some definitions

The closure temperature of a geochronolgical system may be defined as the temperature at the time corresponding to the apparent age. . . .

The temperature recorded by a "frozen" chemical system, in which a solid phase in contact with a large reservoir has cooled slowly from high temperatures, is formally identical with geochronological closing temperature

M.H. Dodson (1973), Contrib.Min.Pet., 40, 259-274

Temperature dependence of diffusion coefficient

Diffusion coefficient usually follows the Arrhenius relation

$$D(T) = D_\infty e^{\frac{-E}{RT}},$$

where D_∞ is the diffusion coefficient for $RT >> E$, i.e. for infinitely high temperature. If temperature varies with time, $T = T(t)$:

$$D(t) = D_\infty e^{\frac{-E}{RT(t)}}$$

and the diffusion equation becomes

$$\frac{\partial c}{\partial t} = D(t)\frac{\partial^2 c}{\partial x^2}$$

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Transformation of the time variable

Use $T_0 = T(t = 0)$, then:

$$D(t) = D_0 \ \exp\left[-\frac{E}{R}\left(\frac{1}{T(t)} - \frac{1}{T_0}\right)\right],$$

where D_0 is D at T_0. Introduce $\zeta(t)$ to scale D to the correct value at time t

$$D(t) = D_0 \, \zeta(t)$$

Transformed (*compressed*) time is then defined as:

$$t' = \int_0^t \zeta(t) \, dt$$

or replacing for $\zeta(t)$

$$t' = \int_0^t \exp\left[-\frac{E}{R}\left(\frac{1}{T(t)} - \frac{1}{T_0}\right)\right] dt$$

Transformation of the time variable

by differentiation we obtain

$$dt' = \zeta(t)\, dt$$

The diffusion equation then becomes

$$\frac{\partial c}{\partial t} = D_0\, \zeta(t) \frac{\partial^2 c}{\partial x^2},$$

dividing both sides by $\zeta(t)$ and using $dt' = \zeta(t)\, dt$ yields:

$$\frac{\partial c}{\partial t'} = D_0 \frac{\partial^2 c}{\partial x^2},$$

i.e. the problem is reduced to a *standard* diffusion problem with constant diffusion coefficient.

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Cooling History

Let T decrease monotonously from T_0 at a constat cooling rate s so that:

$$T(t) = \frac{T_0}{1 + (st/T_0)}$$

The time dependence of D may then be expressed as:

$$D(t) = D_0 \ \exp\left[-\frac{Est}{RT_0^2}\right]$$

Let $\gamma = Es/RT_0^2$ then this becomes

$$D(t) = D_0 e^{-\gamma t},$$

and

$$t' = \frac{1}{\gamma}\left(1 - e^{-\gamma t}\right).$$

t' can not increase to infinity but is limited to a finite value,

$$\lim_{t\to\infty}(t') = 1/\gamma.$$

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Atomistic interpretation of "cooling" / "freezing"

For a small time interval $d\tau$ the mean squared distance traveled by a particle in a small time interval $d\tau$ is $2D_\tau d\tau$ (Einstein equation). The total mean squared distance traveled after time t is

$$\left(X^2\right) = \int_0^t 2D_\tau d\tau$$

given cooling at a constant cooling rate and inserting for D_τ yields:

$$\left(X^2\right) = 2D_0 \frac{1}{\gamma}\left(1 - e^{-\gamma t}\right),$$

The limiting distance traveled by a particle after $t \to \infty$ is then:

$$\left(X^2\right) = 2D_0 \frac{1}{\gamma} = 2D_\infty e^{-\frac{E}{RT_0}} \frac{RT_0^2}{Es}.$$

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Atomistic interpretation of “cooling” / “freezing”

Let a be a typical diffusion distance in a geological process , then the closuretemperature, T_c, may be obtained by finding the minimum initial temperature, T_0, which gives a diffusion distance of a :

$$a^2 = \frac{2D_\infty RT_c^2}{Es} e^{-\frac{E}{RT_c}}$$

If $T_0 > T_c$, then the mean squared distance traveled by a particle $> a^2$, if $T_0 < T_c$, then the mean squared distance traveled $< a^2$ and the mineral grain acts as a *closed system*. Rearrangement gives:

$$T_c = \frac{E/R}{\ln\left[2D_\infty RT_c^2/a^2 Es\right]}$$

This may be iterated to obtain T_c.

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