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By J. T. Bracken and F. E. Senftle

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When diffusion occurs in a solid system containing two or more isotopes of a given element, a change in the isotopic ratio within the body would be expected because of the difference in mass of the isotopes. For some geological problems it is desired to obtain an indication of the average isotopic fractionation within a body, such as a crystal, due to diffusion of nuclides of different masses. To reduce the problem to simplicity an ideal case is assumed.

A hypothetical homogeneous sphere of solvent material is embedded in an infinite homogeneous medium of the same solvent material. Within the sphere at time t equal zero all the solute atoms are homogeneously distributed, i.e., the sphere is treated as an instantaneous source. Diffusion of the solute proceeds into the exterior medium at a uniform rate in all directions and the diffusion coefficient D, is assumed to be independent of concentration and the same both inside and outside of the sphere.

The concentration, Cr, as a function of the radius a of the hypothetical sphere, the time t, and the diffusion coefficient D, at any distance $r < a$, is

$$C_r = \frac{3 Q_0}{4 a^3 \pi^{3/2}} \left\{ \int_0^{\frac{r+a}{2\sqrt{Dt}}} e^{-y^2} dy - \int_0^{\frac{r-a}{2\sqrt{Dt}}} e^{-y^2} dy - \frac{\sqrt{Dt}}{r} \left(e^{-\frac{(r-a)^2}{4Dt}} - e^{-\frac{(r+a)^2}{4Dt}} \right) \right\} \quad \text{............ (1)}$$

where Q_o is the original quantity of the diffusing substance (Barrer, 1951; Carslaw and Jaeger, 1947).

If we now consider Q as the total quantity of an isotope of a given mass within the sphere, then

$$Q = 4\pi \int_0^a r^2 C_r \, dr \qquad \text{............ (2)}$$

Integrating and substituting (1) in (2), one obtains

$$Q = \frac{3Q_o}{a^3\sqrt{\pi}} \left[\frac{\sqrt{\pi}}{2} \left(\int_0^a r^2 \operatorname{erf} \frac{r+a}{2\sqrt{Dt}} \, dr - \int_0^a r^2 \operatorname{erf} \frac{r-a}{2\sqrt{Dt}} \, dr \right) + \sqrt{Dt} \left(\int_0^a r e^{-\frac{(r+a)^2}{4Dt}} dr - \int_0^a r e^{-\frac{(r-a)^2}{4Dt}} dr \right) \right] \qquad \text{............ (3)}$$

Simplifying, it can be shown that

$$Q = Q_o \left[\operatorname{erf} \frac{a}{\sqrt{Dt}} + \frac{2}{\sqrt{\pi}} \left(\frac{\sqrt{Dt}}{a} \right)^3 \left(1 - e^{-\frac{a^2}{Dt}} \right) - \frac{\sqrt{Dt}}{a\sqrt{\pi}} \left(3 - e^{-\frac{a^2}{Dt}} \right) \right] \qquad \text{............ (4)}$$

This equation satisfies the boundary conditions $Q = Q_o$ for D or $t = o$; and $Q = o$ when D or $t = \infty$; and Q has values of $Q_o \geq Q \geq 0$ for all positive values of Dt and a.

Since for all practical purposes $D_L = \sqrt{M_H/M_L}\ D_H = k\ D_H$, where the subscripts L and H refer to the masses, M, of light and heavy isotopes, an expression for the isotopic fractionation factor within a spherical body as a function of a, D, and t can be obtained. Thus

$$f = \frac{Q_L\, Q_{H_o}}{Q_H\, Q_{L_o}} = \frac{\operatorname{erf}\frac{a}{\sqrt{kDt}} + \frac{2}{\sqrt{\pi}}\left(\frac{\sqrt{kDt}}{a}\right)^3\left(1-e^{-\frac{a^2}{kDt}}\right) - \frac{\sqrt{kDt}}{a\sqrt{\pi}}\left(3-e^{-\frac{a^2}{kDt}}\right)}{\operatorname{erf}\frac{a}{\sqrt{Dt}} + \frac{2}{\sqrt{\pi}}\left(\frac{\sqrt{Dt}}{a}\right)^3\left(1-e^{-\frac{a^2}{Dt}}\right) - \frac{\sqrt{Dt}}{a\sqrt{\pi}}\left(3-e^{-\frac{a^2}{Dt}}\right)} \qquad (5)$$

The mean percent enrichment, $\bar{S}$, within the sphere, is defined as

$$S = (1-f)\cdot 10^2 \qquad (6)$$

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