Chapter 2 Compartmental Models

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0.1 Olduvai Gorge

0.1.1 Background

Olduvai Gorge, in Kenya, cuts through volcanic flows, tuff (volcanic ash), and sedimentary deposits. It is the site of bones and artefacts of early hominids, considered by some to be precursors of man. In 1959, Mary and Louis Leakey uncovered a fossil hominid skull and primitive stone tools of obviously great age, older by far than any hominid remains found up to that time. Carbon-14 dating methods being inappropriate for a specimen of that age and nature, dating had to be based on the ages of the underlying and overlying volcanic strata.

The method used was that of potassium-argon decay. The potassium-argon clock is an accumulation clock, in contrast to the 14C dating method. The potassium-argon method depends on measuring the accumulation of 'daughter' argon atoms, which are decay products of radioactive potassium atoms. Specifically, potassium-40 (40 K) decays to argon (40 Ar) and to Calcium-40 (40 Ca) by the branching cascade illustrated below in Figure. Potassium decays to calcium by emitting a β particle (i.e. an electron). Some of the potassium atoms, however, decay to argon by capturing an extra-nuclear electron and emitting a γ particle.

The rate equations for this decay process may be written in terms of K(t), A(t) and C(t), the potassium, argon and calcium in the sample of rock:

$$K' = -(k1 + k2)K, A' = k1K, C' = k2K$$
(1)

where

$$k_1 = 5.76 \times 10^{-11} year^{-1}, k_2 = 4.85 \times 10^{-10} year^{-1}$$
 (2)

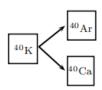


Figure 1: Compartment Diagram

0.1.2 Solve the system to find K(t), A(t) and C(t)

We want to solve K'=-(k1+k2)K, then we multiply $e^{(k1+k2)t}$ on both sides. The equation becomes

$$e^{-(k_1+k_2)t}k + (k_1+k_2)e^{-(k_1+k_2)t}K = 0, (3)$$

that is

$$(e^{-(k_1+k_2)t}K)' = 0, (4)$$

$$e^{-(k_1+k_2)t}K = c, c = K(0) = k_0, (5)$$

$$K(t) = k_0 e^{-(k_1 + k_2)t}, (6)$$

Similarly, we have

$$A(t) = \frac{-1}{k_3} k_1 k_0 e^{-(k_3)t} + \frac{k_1 k_0}{k_3},\tag{7}$$

$$C(t) = \frac{-1}{k_3} k_2 k_0 e^{-(k_3)t} + \frac{k_2 k_0}{k_3}, \tag{8}$$

0.1.3 Basic Induction

1. For all $t \geq 0$,

$$K(t) + A(t) + C(t) = k_0,$$
 (9)

since the left hand side of equation is

$$\frac{-1}{k_1 + k_2} k_1 k_0 e^{-(k_1 + k_2)t} + \frac{k_1 k_0}{k_1 + k_2} + \frac{-1}{k_1 + k_2} k_2 k_0 e^{-(k_1 + k_2)t} + \frac{k_2 k_0}{k_1 + k_2} + k_0 e^{-(k_1 + k_2)t}, \tag{10}$$

it can be written as

$$\frac{-1(k1+k2)}{k_1+k_2}k_0e^{-(k_1+k_2)t} + k_0e^{-(k_1+k_2)t} + \frac{(k_1+k_2)k_0}{k_1+k_2},\tag{11}$$

which is directly equal to k_0

2. For $t \to \infty$,

$$K(t) \to 0, A(t) \to \frac{k_1 k_0}{k_3}, C(t) \to \frac{k_2 k_0}{k_3},$$
 (12)

because the power exponent tends to negative infinity when t tends to positive infinity. Then K(t) tends to 0, while A(t) tends to $\frac{k_1k_0}{k_1+k_2}=\frac{k_1k_0}{k_3}$, B(t) tends to $\frac{k_2k_0}{k_1+k_2}=\frac{k_2k_0}{k_3}$

3.

$$\frac{A}{K} = \frac{k_1}{k_3} (e^{k_3 t} - 1),\tag{13}$$

since

$$\frac{A(t)}{K(t)} = \left(\frac{-1}{k_1 + k_2} k_1 k_0 e^{-(k_1 + k_2)t} + \frac{k_1 k_0}{k_1 + k_2}\right) / k_0 e^{-(k_1 + k_2)t},\tag{14}$$

multiply both numerators and denominators by $(k_1 + k_2)e^{(k_1+k_2)t}$, the right hand side can be simplify to

$$\frac{-k_1k_0 + k_1k_0e^{k_3t}}{k_0k_3},\tag{15}$$

which is exactly $\frac{k_1}{k_3}(e^{k_3t}-1)$.

4. the age of the sample in years is

$$t = \frac{1}{k_3} \ln[(\frac{k_3 A}{k_1 K}) + 1],\tag{16}$$

obtain from simply transformation of (13), in more detail, first multiply $frack_3k_1$ on both sides, then plus 1 on both sides:

$$\frac{k_3 A}{k_1 K} + 1 = e^{k_3 t},\tag{17}$$

then take ln on both sides, finally divide both sides by k_3 . Then we get equation (16).

0.1.4 Implement

When the actual measurements were made at the University of California at Berkeley, the age of the volcanic material (and thus the age of the bones) was estimated to be 1.75 million years. We can use our induction to find the value of the measured ratio A/K.

$$\frac{A}{K} = \frac{k_1}{k_3} (e^{k_3 t} - 1), t = 1.75, k_1 = 5.76 \times 10^{-6}, k_2 = 4.85 \times 10^{-5},$$
(18)

$$\frac{A}{K} = \frac{5.76 \times 10^{-6}}{54.26 \times 10^{-6}} (e^{54.26 \times 10^{-6} \times 1.75} - 1), \tag{19}$$

$$\frac{A}{K} \approx 1.008 \times 10^{-6}$$
 (20)

0.2 Smoke In The Bar

0.2.1 Background

A public bar opens at 6 p.m. and is rapidly filled with clients of whom the majority are smokers. The bar is equipped with ventilators that exchange the smoke-air mixture with fresh air.

Cigarette smoke contains 4% carbon monoxide and a prolonged exposure to a concentration of more than 0.012% can be fatal. The bar has a floor area of 20 m by 15 m, and a height of 4 m. It is estimated that smoke enters the room at a constant rate of $0.006~m^3$ /min, and that the ventilators remove the mixture of smoke and air at 10 times the rate at which smoke is produced.

The problem is to establish a good time to leave the bar, that is, sometime before the concentration of carbon monoxide reaches the lethal limit.

0.2.2 Model Establish

Balance law leads us to the word equation, for the volume of carbon monoxide in the bar,

$$\begin{cases} rate \ of \ change \\ of \ concentration \\ of \ carbon \ monoxide \end{cases} = \begin{cases} rate \ of \\ cincentration \ of \\ carbon \ monoxide \ in \end{cases} - \begin{cases} rate \ of \\ concentration \ of \\ carbon \ monoxide \ out \end{cases}$$

$$\frac{dX}{dt} = \frac{0.006 \times 0.04}{20 \times 15 \times 4} - \frac{X \times 10 \times 0.006}{20 \times 15 \times 4}, X(0) = 0$$

where X represents the concentration of carbon monoxide in gas mixture and t represents the time in minutes after the bar is opened. The exact solution of this equation is $X(t) = 0.004 - 0.004 \times exp(-0.0005t)$. We can also solve it by numerical method. Use Newtons Method, the solution is shown in following figure.

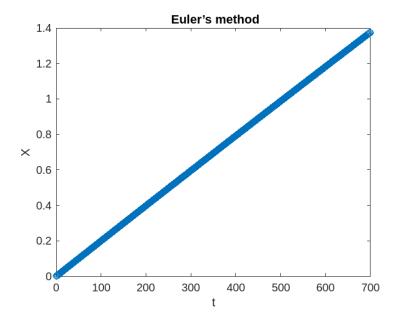


Figure 2: Shows the trend of carbon monoxide concentration in the bar over time

To find the good time to leave the bar, we want to find that t s.t. X(t) = 0.00012.

Obtaining by this equation, we get t=609.18(min), which is about 10 hours. As the public bar opens at 6 p.m. customers are suggested to leave before tomorrow 4 a.m.

0.3 Appendix

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Code for solving the ode problem by Euler's method: time\ span = 0.0.1.700; delta\ t = 0.1; time = time\ span; X = zeros(size(time)); X(1) = 0; for\ i = 1.length(time)-1 dXdt = 0.0000002 - 0.00005*X(i); X(i+1) = X(i) + delta\ t\ *\ dXdt; end plot(time,\ X,\ '-o'); title('\ Euler's\ method'); xlabel('t'); ylabel('X');
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