Measuring and Modelling Diffusion

Blerta and Marc and others! :-)

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Abstract

The movement of compounds in the environment is driven by two processes, advection and diffusion. Of course, these processes occur in three dimensions, but for this class we'll begin with one dimensional processes before getting to more complecated examples.

Introduction

The movement of contaminants through a media (e.g. air, water, and soil) is complex and difficult to predict.

In general, pollutants move in two ways: advection and dispersion. Advection is the bulk flow of materials that are "carried" by wind patterns, water currents, or groundwater flow paths. Dispersion is the spreading of the chemical via localizied mixing or diffusion. As you might guess, descriptions of advection and dispersion depend on the scale of interest, and can be described by a variety of equations.

Pre-lab Activity

Pre-assessment: What do you know about diffusion?

Conceptual Models of Diffusion

Preparing for the Lab

What can you do to prepare for the lab? Great question.

I have been thinking about this for a few weeks and have some suggestions.

1. Decide how you will make the standard curve before coming to class.
2. Review the recipe to make the agarose and write it out in your laboratory book.
3. Decide how you will sample your agar (spatially) and
4. create some tables to record the data in the lab book before class.
5. The bulk density of the agar is 1.5 g/ml. That means for every 1 gram, you will have a volume of 0.66 mL. You should check this to see how I get this. You will be diluting this volume as you heat

them to get the dye into the solution. How will you back calculate the concentration of the dye given a dilution effect in the test tubes that you melt the agar in?

6. What are the possible interferences that you should consider? IMPORTANT: What blanks should you be sure to do?

Laboratory Methods

Preparing Agarose and Sampling Methods

Agarose gels are prepared by adding the desired volume...

The resulting slurry was heated to 90∘C until complete dissolution of agarose, and then slowly cooled. Before gelation, the viscous agarose solution was cast, then slowly cooled at room temperature. The cast are in circular petri dishes (40 cm in diameter).

Samples will be taken from the petri dishes with an exacto knife. Try to sample 1 cm^3. Record the two distances of the agar sampled – and weight sample to obtain a volume (via density).

Equipment

- Precision Balances
- 20 ml pipettes
- 50 ml beaker
- Weighing boats
- Distilled water
- Saran wrap
- Spec 20?

Previous Results

The following are images of notes from a previous lab: I still need to work on translating these into something I can translate. These are over 5 years old and because the results were so ambiguous, I think I never got around to writing this out.

Here are the results: without the T_0 I was completely lost of how to deal with this. But in reality, these are the kind of data we get with groundwater sampling...so, it must be trivial!

Conc	Distance from Center	Mass
0.035	1	5
0.019	7	5.2
0.001	11	5.3
0.001	15	4.8

Table 1: Results from a Test

Variations on the Theme

I wonder if we tilt the petri dishes? This would create a preferential flow down gradient. Perhaps a slight tilt?

Assessment

Diffusion Derivation

a.) From 9.3, Special Case 2, we know that if $A(x,t) = \bar{A}(x) \neq 0$ (if area does not change with time), then the equation can be written as

$$\frac{\partial c(x,t)}{\partial t} = -\frac{1}{\bar{A}(x)}\frac{\partial}{\partial x}[J(x,t)\bar{A}(x)] \pm \sigma(x,t) \tag{1}$$

We now need to find an equation for $\bar{A}(x)$. Since arc length equals radius times angle, we get

$$\bar{A}(r) = \theta r h \tag{2}$$

where θ is the angle of the arc, r is radial distance, and h is height of the section. Therefore we get the equation

$$\frac{\partial c(r,t)}{\partial t} = -\frac{1}{\theta r h}\frac{\partial}{\partial r}[J(r,t)\theta r h] \pm \sigma(r,t) \tag{3}$$

Since θ and h are constants, we can factor them out to get

$$\frac{\partial c(r,t)}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}[J(r,t) r] \pm \sigma(r,t) \tag{4}$$

b) Extending the principle applied in part (a), we first need to find $\bar{A}(R)$. Since θ is small, we can approximate cross sectional area by taking horizontal arc length times vertical arc length. Therefore we get the equation

$$\bar{A}(R) = \theta_1 \theta_2 R^2 \tag{5}$$

where θ_1 is the horizontal angle of the arc, θ_2 is the vertical angle of the arc, and R is radial distance. Combining this with equation (1) from above, we get

$$\frac{\partial c(R,t)}{\partial t} = -\frac{1}{\theta_1\theta_2 R^2}\frac{\partial}{\partial R}[J(R,t)\theta_1\theta_2 R^2] \pm \sigma(R,t) \tag{6}$$

Since θ_1 and θ_2 are constants, we can simplify the equation as such:

$$\frac{\partial c(R,t)}{\partial t} = -\frac{1}{R^2}\frac{\partial}{\partial R}[J(R,t)R^2] \pm \sigma(R,t) \tag{7}$$

c) Part A: In order to obtain the equations in 9.5, we apply Fick's law:

$$J = -\mathcal{D}\nabla c \tag{8}$$

In this case, we use the one-dimensional version:

$$J = -\mathcal{D}\frac{\partial c}{\partial x} \tag{9}$$

Applying this to equation (4), we get

$$\frac{\partial c(r,t)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}[\mathcal{D}\frac{\partial c}{\partial r}r] \pm \sigma(r,t) \tag{10}$$

Simplifying, and assuming that no particles are created or eliminated at the source, we get:

$$\frac{\partial c(r,t)}{\partial t} = \frac{\mathcal{D}}{r}\frac{\partial}{\partial r}(\frac{\partial c}{\partial r}r) \tag{11}$$

Part B: Once again, we apply Fick's law in one dimension to get

$$\frac{\partial c(R,t)}{\partial t} = \frac{1}{R^2}\frac{\partial}{\partial R}[\mathcal{D}\frac{\partial c}{\partial R}R^2] \pm \sigma(R,t) \tag{12}$$

We again simplify, assuming no particles are created or destroyed at the source.

$$\frac{\partial c(R,t)}{\partial t} = \frac{\mathcal{D}}{R^2}\frac{\partial}{\partial R}(\frac{\partial c}{\partial R}R^2) \tag{13}$$

Chang 1997 Key Points

Data

- Size of halos measured with a ruler over constant time intervals
- Experiment repeated three times to calculate average values used in model

Methodology

- Mathematical model formed using Fick's law
- c(r,t) = lipase concentration as a function of time and radial distance
- Used regression analysis to fit hindered diffusion coefficients and threshold values of lipase concentration as parameters. The finite difference method outlined in Constantinides, 1987 was used specifically.
- Amount of lipase in plate at each time calculated by numerical integration. The total amount of lipase varied by 2.5%, confirming the appropriateness of the mathematical model used.

Discretization

Fick's second law of molecular diffusion, expressed in cylindrical coordinates.

$$\begin{aligned}\frac{\partial C}{\partial t} &= D\Delta^2 C \\ &= D(\frac{1}{r}\frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial r^2})\end{aligned}$$

Initial conditions:

$$\begin{cases} C = C_0 & \text{for } R_w < r < R_r \\ C = 0 & \text{for } r < R_w \ \& \ R_r < r \end{cases} \tag{14}$$

where D is the effective hindered diffusion coefficient, C_0 is the feed enzyme concentration, R_w is the radius of the well, and R_r is the outer radius of the absorption ring. The lipase concentration as a function of time and radial distance can be solved using the finite difference method.

$$\frac{1}{\Delta t}(C_{i,j+1} - C_{i,j}) = [\frac{1}{i\Delta r}\frac{D}{2\Delta r}(C_{i+1,j} - C_{i-1,j}) + \frac{D}{\Delta r^2}(C_{i+1,j} - 2C_{i,j} + C_{i-1,j})] \tag{15}$$

$$\frac{1}{\Delta t}C_{i,j+1} = \frac{1}{\Delta t}C_{i,j} - \frac{2D}{\Delta r^2}C_{i,j} + \frac{D}{2i\Delta r^2}(C_{i+1,j} - C_{i-1,j}) + \frac{D}{\Delta r^2}(C_{i+1,j} + C_{i-1,j}) \tag{16}$$

$$C_{i,j+1} = (1 - \frac{2D\Delta t}{\Delta r^2})C_{i,j} + \frac{D\Delta t}{\Delta r^2}[(\frac{1}{2i} + 1)C_{i+1,j} - (\frac{1}{2i} - 1)C_{i-1,j}] \tag{17}$$

For convergence, to hold:

$$\frac{D\Delta t}{\Delta r^2} \leq \frac{1}{2} \tag{18}$$

Lastly, the amount of lipase can be calculated using

$$A = \int_{R_w}^{R_r} 2\pi r l C(r)\ dr \tag{19}$$

where A is the total amount of lipase in terms of enzyme activity, R_w and R_h are the radius of well and halo, respectively, $C(r)$ is the concentration at the radial distance of r, and l is the thickness of agar plate.