Diffusion at Work
An Interactive Simulation

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PURPOSE OF ACTIVITY

The goal of this activity is to help students better understand the nonintuitive concept of diffusion and introduce them to a variety of diffusion-related processes in the ocean. As part of this activity, students also practice data collection and statistical analysis (e.g., average, variance, and probability distribution functions). This activity is also used as an introduction for a subsequent lesson on stirring and mixing.

AUDIENCE

The activity is designed for undergraduate marine sciences students, but it is also appropriate for biology, chemistry, and lower-level engineering students. The content can be easily modified to suit graduate or high school students. A version of this activity was evaluated in an upper-level undergraduate course at the University of Maine ("Teaching Sciences by Ocean Inquiry;" http://misclab.umeoce.maine.edu/boss/classes/SMS_491_2007/SMS_491_2007_index.htm). The course targeted science majors interested in education and was designed to introduce students to inquiry-based teaching strategies with examples from marine sciences. The diffusion activity was presented as an example of using simulations in science education.

BACKGROUND

Diffusion is a fundamental process central to understanding transport phenomena and mixing processes in the water column and sediments. It describes the dispersion of molecules

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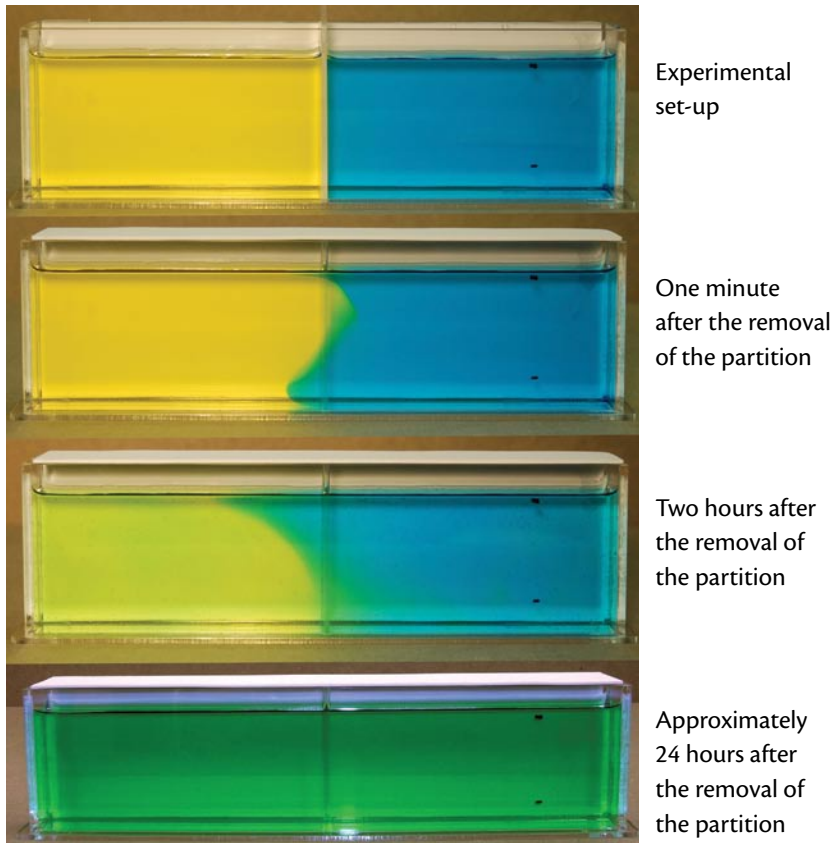
or small particles due to their random (Brownian) motion and the resultant net migration of material from regions of high concentration to regions of low concentration. Stirring (where material gets stretched and folded) expands the area available for diffusion to occur, resulting in enhanced mixing compared to that due to molecular diffusion alone. This helps explain why materials such as milk in coffee diffuse orders of magnitude faster than one would predict based on their molecular diffusion coefficients.

When teaching about diffusion, one can take the macroscopic approach, introducing Fick's law and its mathematical expression that describes the net movement of molecules or small particles across concentration gradients (see Crank, 1980, for a comprehensive treatment). Alternatively, one can approach diffusion from a microscopic perspective by introducing the concept of random walk, which refers to the random motion of individual molecules or particles caused by their thermal kinetic energy. For comprehensive treatments of random walks and diffusion, we refer the reader to Einstein (1956), Taylor (1921), Berg (1983), and Denny and Gaines (2002).

Here, we present two activities: (1) a class demonstration, used as a macroscopic representation of diffusion, and (2) an interactive student simulation that introduces the concepts of a one-dimensional random walk (based on Taylor, 1921) and a biased random walk. We follow these activities with a discussion linking the microscopic process to the macroscopic phenomena of diffusion, and we present related oceanographic examples.

DESCRIPTION OF THE ACTIVITY
Macroscopic Representation of Diffusion

Illustrating molecular diffusion in water without creating convection due to physical disturbance, density flows, or thermal convection is very difficult in a common classroom or lab set-

Experimental set-up

One minute after the removal of the partition

Two hours after the removal of the partition

Approximately 24 hours after the removal of the partition

Figure 1. A demonstration of mixing dominated by molecular diffusion.

initial stirring to slow mixing as time progresses, this activity allows students to gain some appreciation for the slow rate of molecular diffusion. We initiate this demonstration at the beginning of the class and refer back to it at the middle and end of the class period.

Microscopic Representation of Diffusion: One-Dimensional Random Walk

This activity is designed to simulate diffusive spreading in one dimension and follows the rules of a random walk described by Taylor (1921), Berg (1983), and Denny and Gaines (2002). Each student represents a particle that moves independently of all the other particles (students) with an equal probability of going to the right or left in each simulation step. Each simulation step represents one time step (δt). For this activity, you will need a tiled area, which can be a hall or a room with large tiles, or you can use a lot or a field on which you can mark lines. Rows of tiles (or lines) should be numbered (-8, -7, -1, 0, 1…7, 8) prior to class. Each row of tiles or interval represents one spatial step (Δx). Give each student a coin, and have them line up on the row of tiles (or the line) marked with "0" (position $x = 0$; Figure 2), representing a high concentration of molecules at the origin ($t = 0$). At the beginning of the activity, assign a student to record the location of each "particle" (student) after each time step. Having a portable computer with a spreadsheet prepared in advance will save time (see Table 1). Ask all the other students to flip their coins and move one tile/line to the right (if heads), or one tile/line to the left (if tails). The new position is the position at time step $t = 1$. Repeat the process for about 16 time steps, where each coin flip followed by a one-tile move to the right or to the left is defined as one step. Ask the students to return to the original row of tiles and repeat the entire experiment until you obtain at least 20 independent realizations. (Note: A small class may need to repeat the entire simulation several times, whereas a large class may get sufficient realizations without repeating the process.) Have the students summarize the recorded data in a table (see Table 1).

ting. This demonstration is a qualitative representation of time scales associated with mixing resulting from both stirring and molecular diffusion. For this demonstration, we use a rectangular tank divided by a partition that separates water stained with two food colors (Figure 1, top panel); we found that yellow and blue provide the best display. The tank was purchased from sciencekit.com part # WW4702001. At the beginning of the demonstration, the partition is removed carefully and the students observe the rate of mixing by following changes in the distribution of green water formed when the two fluids mix (Figure 1). Removal of the partition initially generates a small amount of physical stirring with accompanying enhanced mixing. As time passes, without additional stirring, the two fluids mix very slowly due to molecular diffusion. Placing a cover on top of the tank helps to reduce convective effects from evaporation, air movement, or temperature changes, so that during a typical class period molecular diffusion remains a dominant mixing process. By contrasting rapid mixing associated with

Table 1. A summary table of the position of each student at each time step.

	Student 1	Student 2	Student 3	Student 4	And so on...
Position at t = 0	0	0	0	0	
Position at t = 1	1	-1	1	1	
Position at t = 2	0	-2	2	0	
Position at t = 16	6	-2	-5	0	

Students may proceed with calculations in class or as a homework assignment. Have the spreadsheet projected on the screen or have the students copy the data to their computers and work in small groups. Ask students to calculate the average position of all particles and the deviation from the mean position at each simulation step (in the form of standard deviation, variance, or the average of the squares of the particle's location) and plot them as a function of time steps. The standard error of the mean may be used to determine whether the mean position at each time step is significantly different from zero. This activity will demonstrate (if enough realizations have been collected) that although most individual particles (students) moved away from the origin, the mean position of the particles does not change significantly from one step to the next and does not move away from the origin ($x = 0$). The spread of the particles (i.e., deviation from the mean), however, increases with time.

As an alternative to telling students what parameters to calculate and plot, an inquiry-based approach, focused on the following questions, will require students to determine the appropriate analyses:

1. How does the mean position of the participants change as a function of time? How can this be determined with the available data?
2. How do the particles spread away from the initial position as a function of time? What mathematical construct can be used to describe the dispersion of particles away from their mean position?

One-Dimensional Biased Random Walk

A biased random walk emphasizes how organisms may drift toward a favorable condition even if they cannot control their direction of motion. Some motile bacteria, for example, use fla- gellar motion. Due to their propulsion mechanism, they must occasionally unwind their flagella, causing them to change direction ("tumble"). As cells swim toward a favorable food source, their tumbling frequency decreases, resulting in longer "runs" in a favorable direction and a net drift towards the attractor (e.g., Berg, 1983). Another example of a biased random walk is the movement of small particles in a gravitational or a magnetic field.

To demonstrate a biased random walk, repeat the simulation described above for the one-dimensional random walk. In this activity, however, a step consists of tossing the coin and moving one tile to the right (if heads) or two tiles to the left (if tails). Because a movement may consist of two tiles at a time, you will need to increase the domain of the experiment. Have a student monitor the position of each "particle" (student) at each time step, and proceed with statistical analysis as described above. Ask students to compare and contrast the two cases.

General Comments

While this activity may seem simplistic and time-consuming, students feedback indicates that it was useful and illuminating. Their own movement simulated molecules and demonstrated to them the connection between microscopic motion and macroscopic distribution as well as the independence of individual molecules in their motion (e.g., two-particle dispersion). Students in our class had learned about diffusion in previous chemistry classes but felt that this activity improved their understanding of the process. As with any other simulation, it is important to note, in a follow-up discussion, where the analogy fails (e.g., molecules do not all move at the same speed). The duration of the activity depends on the size of the class; our experience suggests you should allocate 20–30 minutes for the simulation (not including data analysis and discussion).

| 1. Line-up (t = 0) | 2. Start flipping (t = 1) | 3. Diffusion at work (t = 16) |

Figure 2. Physical simulation of random walk representing microscopic diffusion.

Linking the Microscopic and Macroscopic Descriptions of Turbulence

With advanced students and if time permits, one can link the time step and step size to the diffusion coefficient (e.g., following the analysis in Taylor, 1921; Berg, 1983; or Denny and Gaines, 2002). Students should calculate the mean square displacement ($<x^2>$) as an index of dispersion at each step (n), which represents a time interval (δt). It follows that the mean square displacement increases with n, and the relationship for diffusion in one dimension is given by $<x^2> = 2D\delta t$, where D is the diffusion coefficient (D = $1/2<x^2>$ / δt). The diffusion coefficient characterizes the migration of a given kind of particle in a given medium and temperature and is a function of the size and the shape of the molecule. Note that the proportionality coefficient for diffusion is 1/2 for diffusion in one dimension, 1/4 for two dimensions, and 1/6 for diffusion in three dimensions (for details see Berg, 1983, p. 11). Students might first use dimensional analysis alone to derive $D \propto <x^2>$ / δt. With a large class, students can try simulating different initial conditions, for example, no gradient at all or a heavy-side ("step") function, such as a constant concentration at the bottom of a glass overlaid by no molecules.

RELEVANCE TO OCEANOGRAPHY

Diffusion is at the heart of many ocean processes. Because physical and geochemical studies often require estimations of fluxes of heat, momentum, and mass in a concentration field, advection-diffusion models are essential research tools. Diffusion in the ocean operates at many scales. At very small scales, molecular diffusion is the dominant, and often limiting,

transport mechanism by which microorganisms can exchange nutrients and gases with their environments. Examples of other processes that are regulated by molecular diffusion include dissolution of small particles, bacteria-particle dynamics, and chemosensing in aquatic environments. Within sediments, molecular diffusion often dominates the transport of porewater solutes (e.g., Burdige, 2006).

An interesting case where molecular diffusion affects ocean physics is double diffusion. It is considered to be an important process contributing to fluxes of mass, heat, and momentum (for a review, see Ruddick and Gargett, 2003). Double diffusion denotes processes where an initially stable stratified water column becomes unstable. The instability occurs due to the differential diffusion of salt and heat, which largely control density at a given depth (the molecular diffusion of heat is 100 times faster than the molecular diffusion of salts). There are two cases where such instability occurs. One case is associated with less-dense, warm, and salty water overlaying cold, less-saline waters of higher density, producing the phenomena known as salt fingers. A second case occurs when less-dense, fresh, and cold water overlay denser warm and salty waters, resulting in diffusive convection. This process is less common and mostly observed at high latitudes. Movies of laboratory demonstrations of double diffusion can be found at http://www.phys.ocean.dal.ca/programs/doubdiff/labdemos.html.

At larger scales, effects of turbulence on transport and mixing are often parameterized by diffusion with a large eddy diffusion coefficient (Taylor, 1921). The "thermocline problem," which refers to the magnitude of the effective vertical turbulent diffusion coefficient of heat across the thermocline,

is a fascinating example of a scientific pursuit associated with (eddy) diffusion. Vertical (eddy) diffusion is an important process transporting heat and nutrients from/to the upper ocean. Determining how to parameterize the fluxes caused by (eddy) diffusion has been a major challenge in physical oceanography. Munk (1966) proposed a steady, one-dimensional model that balanced upward advection and downward eddy diffusion due to turbulent mixing. The value of the averaged vertical diffusion coefficient obtained ($\sim 10^{-4}$ m^2/s) was based on fitting this balance to observed vertical profiles of temperature below 1000 m. Ledwell et al. (1993, 1998) monitored the dispersion of dye in the upper thermocline (300-m depth) over a period of several years. Their estimate of the vertical eddy diffusion coefficient ($\sim 10^{-5}$ m^2/s), as well as microstructure estimates below 1000-m depth (e.g., Toole et al., 1994; Kunze and Sanford, 1996), was an order of magnitude smaller than that estimated by the one-dimensional, advective-diffusive balance (though two orders of magnitude larger than the molecular diffusion coefficient for heat). This discrepancy has not been resolved (see review by Kunze and Llewellyn Smith, 2003; Kunze et al., 2006, and references therein) and "is one of the big mysteries in oceanography, comparable to the dark matter question in cosmology" (quoting E. Kunze, University of Victoria, *pers. comm.*, 2007).

ADDITIONAL ONLINE RESOURCES

The following list shows links to a two-dimensional, random-walk, computer-aided simulation and a Web site with simulation of Brownian motion. They can be used in class directly following the activity (or as homework) to compare and contrast with the one-dimensional simulation described above and to provide more information on Brownian motion.

- http://www.geocities.com/piratord/browni/Difus.html
- http://lessons.harveyproject.org/development/general/diffusion/simpdiff/simpdiff.html
- http://www.phy.davidson.edu/brownian.html

ACKNOWLEDGEMENTS

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HANDS-ON OCEANOGRAPHY

Hands-On Oceanography provides an opportunity for you to publish teaching materials developed for undergraduate and/or graduate classes in oceanography. Activities include, but are not limited to, computer-based models and laboratory demonstrations that actively engage students (i.e., activities where students have to make decisions, record results, and interpret results). All submissions are peer-reviewed. Publication of teaching materials may contribute to the broader impact of NSF-funded research.

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