DRAFT! Advection, Diffusion & Reaction Modeling

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The movement of compounds in the environment is driven by two processes, advection and diffusion. The compounds are also subject to transformations or reactions. Thus, to monitor the fate and transport of compounds in the environment, we can capitalize on mathematical models that have been used to describe advection, diffusion, and reaction.

Introduction

Fate and Transport Processes

The fate and transport of compounds in the environment is subject to an array of processes. For example, pollutants might carried by the wind (advection) and spread out (dispersion or diffusion). In addition, the pollutant might be transformed into different compounds (reaction). Together, these three processes, advection, diffusion, and reaction (Figure 1).

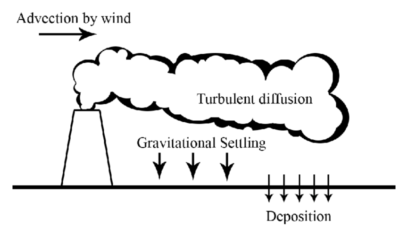


Figure 1: A simple diagram of advection and diffusion that inclues how "solutes" might be deposited downwind of a stationary source if air pollution. At the scale analyzed there, the term turbulant diffusion is different than molecular diffusion, but might be modelled in a similar way.

These three processes have profound implications – they provide the a framework to understand and quantify the fate and transport of pollutants in the environment (Figure 2), the movement of nutrients in the soil, and the movement of solutes in the human body. By understanding of these processes, we have tools to characterize environmental quality and its implications on human and non-human populations. Moreover, by modeling these processes, we can develop more effective policy, regulation, and mitigation strategies.

Because these processes are complex and are often difficult to measure, we rely on models to help us understand the movement of solutes in the environment. These models are based on the fundamental mathematical equations to describe advection, diffusion, and reaction.

The Processes

As an example of the three processes consider a droplet of dye in water as a dose in a solution. The dye will move with the bulk motion of the water (advection), spread out by random molecular motion (diffusion)(Figure 3), and disappear as it reacts with the water (reaction).

Advection and diffusion govern the transport of solutes in the environment. Advection is the transport of a solute by the bulk motion of the fluid. Advection depends on velocity or ν in this session.

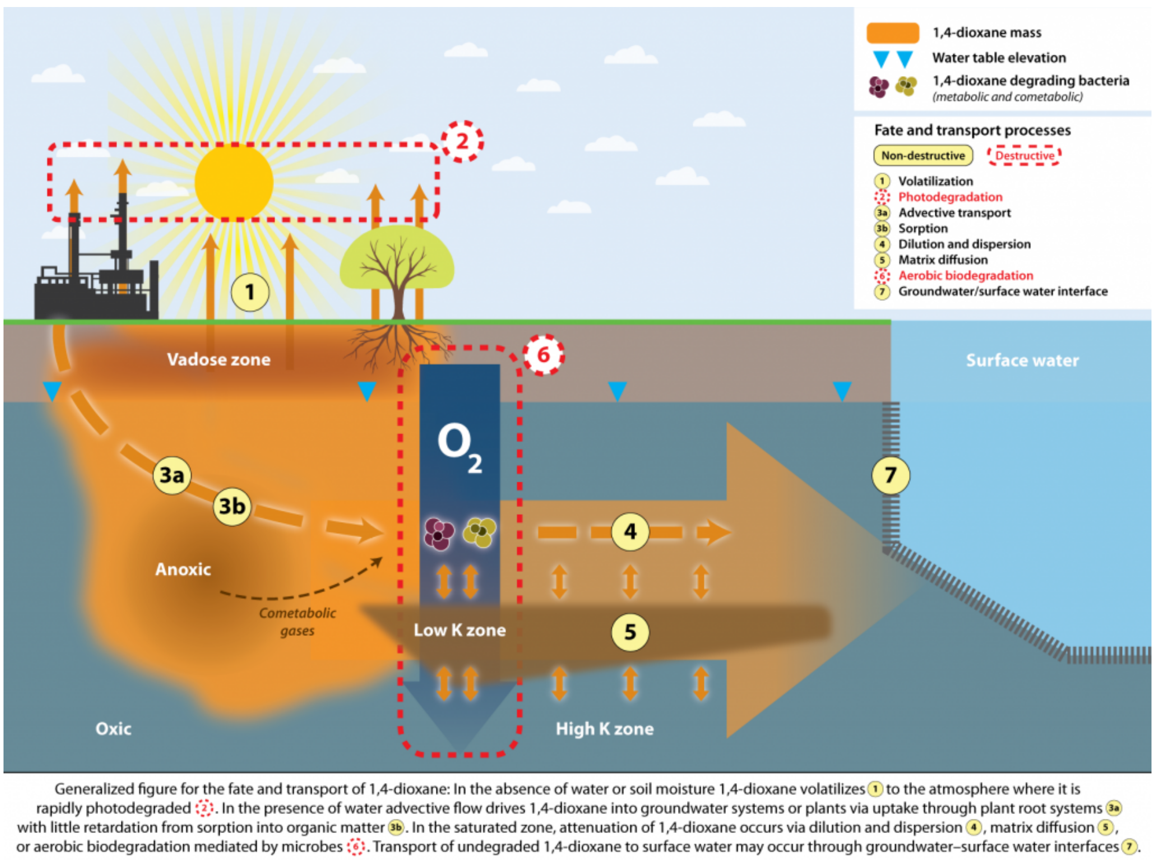


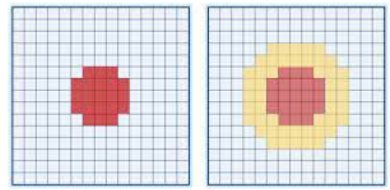
Figure 2: A diagram of the major processes that influence the fate and transport of a dioxane plume from a ce in the environment (Source: `https://14d-1.itrcweb.org/environmental-fate-transport-and-investigative-str` 1,4-Dioxane is often referred to as a "forever" compound.

Diffusion is the transport of a solute by random molecular motion. Diffusion depends on the diffusion coefficient and the concentration gradient or $\frac{\partial^2 C}{\partial x^2}$ in this session. Notice that this is the second derivative.

Reaction is the transformation of a solute into a different compound. Reaction depends on the reaction rate or k in this session.

In the case of air pollution, we are interested in the pollutant in the context of the air – or the media of air (Figure 1). And for air pollution, the chemical transformations are a critical part of our regulatory framework (Figure **??**). In the case of water, we might think about solutes in the water as a media. For example, the movement of a nutrient in a river is driven by the bulk motion of the water (advection) through the water column and the sediments (two types of media) and the random motion of the molecules (diffusion) and the reactions that might occur in the water column and sediments (Figure5).

Figure 3: A simple diagram of 2D diffusion. To solve these equations, we'll use a numerical approach and descretize the media into a grid. We'll then solve the equations for each grid cell.



(a) Initial state (b) One step diffusion

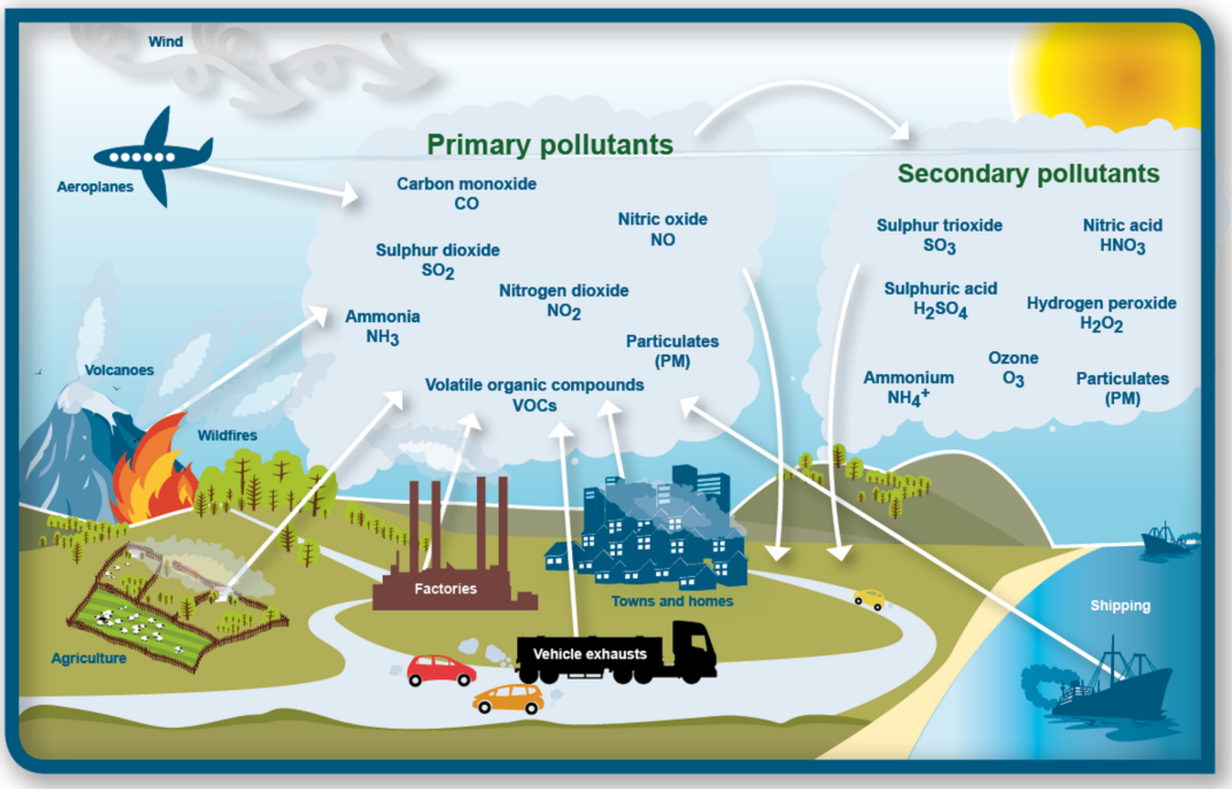


Figure 4: A simple diagram of advection and diffusion in the context of air pollution.

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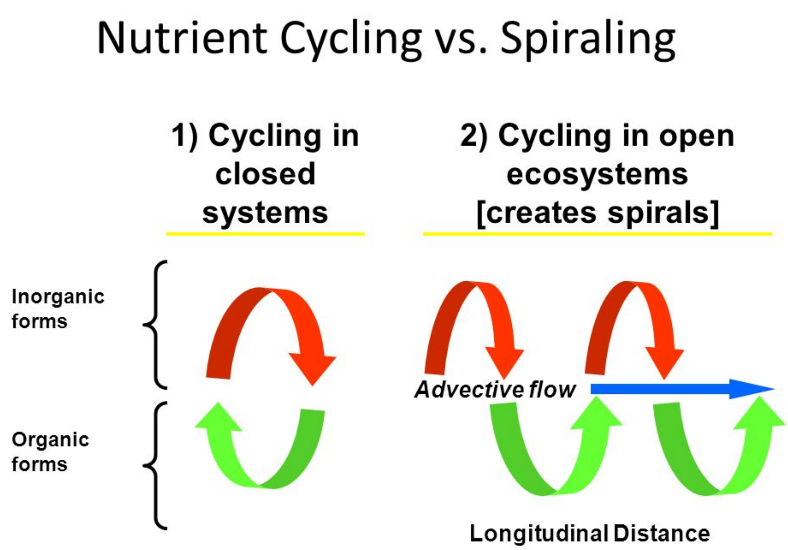

Figure 5: A simple diagram of advection and nutrient reactions (organic substances and inorganic substances) in a river. Although not shown, you might also think about how diffusion might influence the movement of nutrients in the river and in the sediments. The zone where water moves into the sediment bed is called the hyperreic zone. The porosity of the sediments will allow more advective flow that might influence the reaction capacity of solutes in the sediments.

Session Goals

We will not become experts in advection-diffusion-reaction modeling, but we will become familiar with the processes and the equations that describe them. Moreover, we'll see a bit more about how R can be used to model these processes. After this session, I hope you can do the following:

1. Describe the physical processes of advection and diffusion and solute reaction
2. Describe the equations used to model A-D-R.
3. Analyze 1-dimensional movement using advection equations in R.
4. Describe diffusion mathematically
5. Analyze 1-dimensional adveecton-diffusion using R.
6. Appreciate how two-dimensional analysis of advection-diffusion can be modeled in R.

In this session, we'll want to think about the movement of solutes in the porous media, i.e. a soil with air space, sediments with water between the particles. We will refer to the porousity as ξ, which is a proportion between 0 and 1.

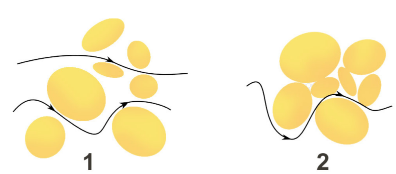

Figure 6: Notice how the porosity of the media can influence the path of the fluid. In ground water, this is measured as permeability and can be used to evaluate the flow chacterstitics in aquifers and oil fields. The permeability is a function of the porosity and the connectivity of the pores.

Equations to Describe Processes

An Equation that Often Creates Anxiety

The advection equation is a partial differential equation that describes the movement of a substance in a fluid. The equation is derived from the conservation of mass. The equation is:

$$-\frac{1}{A_x \xi_x} \cdot \left(\frac{\partial}{\partial x} A_x \cdot \left(-D \cdot \frac{\partial \xi_x C}{\partial x} \right) - \frac{\partial}{\partial x} \left(A_x \cdot v \cdot \xi_x C \right) \right) \tag{1}$$

$$\frac{\partial C}{\partial t} = D_x \frac{partial^2 C}{partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - v_x \frac{\partial C}{\partial x} - \lambda RC \tag{2}$$

Here D is the "diffusion coefficient", ν is the "advection rate" (or velocity), and A_x and ξ are the surface area and volume fraction, respectively.

As you complete the first part of this handout, please do some reflecting:

> What you look at this equation, think about how it makes you feel. It's a bit intimidating, to say the least. But that's only part of the story. I believe these equations, when put in front of is generates anxiety – and this anxiety can be a barrier to learning. While it's easy to claim we can just put this anxiety away seems to be be a disservice and acknoweldgement of our emotional responses. Before moving forward, let's take a moment to acknowledge the anxiety and see where in your body you are feeling that. Take a deep breath and let it out several times before moving forward.

First, let's simplify this to 1-D (in one direction, x).

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - \nu \frac{\partial C}{\partial x} - R \tag{3}$$

Left side: $\frac{\partial C}{\partial t}$

The left side of the equation describes the change in concentration over time. This is the rate of change of the concentration of the solute in the fluid. In steady state, this term is zero, which will use use to model the steady state concentration of the solute in the fluid.

First term on the right side: $D \frac{\partial^2 C}{\partial x^2}$

The first term on the right side of the equation describes the movement of the solute due to diffusion. This is the rate of change of the concentration of the solute in the fluid due to the movement of the solute from areas of high concentration to areas of low concentration.

Second term on the right side: $-\nu \frac{\partial C}{\partial x}$

The second term on the right side of the equation describes the movement of the solute due to advection. This is the rate of change of the concentration of the solute in the fluid due to the movement of the fluid.

Third term on the right side: $-R$

The third term on the right side of the equation describes the rate of change of the concentration of the solute in the fluid due to reactions. This is the rate of change of the concentration of the solute in the fluid due to the reaction of the solute with other compounds in the fluid.

> **Pause for a moment:** Reflect on your emotional state. What are you feeling? Where are you feeling it? Take a deep breath and let it out several times. You have completed the reading for Wednesday's class.

References

https://en.wikipedia.org/wiki/Convection%E2%80%93diffusion_equation

References

Soetaert, K., Meysman, F., and Soetaert, M. K. (2017). Package âĂŸreactranâĂŹ.