At a pristine lake in Ontario, Canada, scientists had been adding low levels of estrogen to the lake and were watching for changes. The levels were approximately equal to the concentration of estrogen found in treated sewage discharge.

The result: fathead minnow populations began to collapse!

Many of the chemicals that we use and release, whether on purpose or by accident, can have severe effects on organisms and ecosystems. To predict the accumulation and levels of contaminants, we can use differential equations.

This video is part of the Differential Equations video series.

Laws that govern a system's properties can be modeled using differential equations.

Hi, my name is David Griffith, and I'm a graduate student in the MIT/Wood's Hole Joint Program in Oceanography and the Department of Civil and Environmental Engineering at MIT.

Before watching this video, you should be familiar with defining control volumes and applying conservation of mass.

After watching this video, you will be able to: Construct a differential equation to estimate the concentration of a chemical in the environment; and Appreciate how informed estimates can help simplify and solve these differential equations.

While everyday chemicals provide a range of benefits to society, they are often released into the environment and can cause unintended harm. Examples include acid rain from smokestack sulfur emissions, toxic groundwater from leaky gas station tanks, and endocrine disruption in fish populations due to treated and raw sewage discharges.

It would be helpful if we could monitor the levels of potentially hazardous chemicals in the environment. But, given the tens of thousands of chemicals in daily use, it shouldn't be surprising that measuring all of them is not practical.

So, what we need is a framework for simplifying a very complex world. We accomplish this through the use of mathematical models, which are simplified versions of reality.

Many models take the form of differential equations, which describe how one variable, like the concentration of a chemical, changes with respect to another variable, like time.

By applying conservation of mass, we can model the change in chemical concentration with time as being equal to the inputs minus the outputs. An input is the rate at which a chemical enters our control volume. An output is the rate at which the chemical leaves the control volume.

To find the inputs and outputs of chemicals into a control volume, the first step is to identify the ways that chemicals enter and leave the control volume. If we think about the estrogen experiment in Ontario, the estrogen entered the lake from the scientist intentionally dumping estrogen from a motorboat and from the fish themselves.

Once released into the lake, there are many ways estrogens can leave the lake. A stream could carry the estrogens out of the lake. Also, physical, chemical, and biological processes within the lake could degrade the estrogens to inactive byproducts.

In my own research, I am interested in the fate of estrogens in the treated sewage that is discharged into Massachusetts Bay.

To start, I had two initial questions: 1) would the estrogen levels in the bay be high enough to detect with our instruments?

And 2) how much water would I need to collect?

To answer these questions, I needed to estimate the concentration of estrogen in the bay.

This is where the differential equation comes in. We can set up the equation by setting the time change in estrogen concentration (dC/dt) equal to inputs minus outputs.

Note that our definition of outputs includes both physical flows and chemical reaction rates. What are the possible inputs? Because Massachusetts Bay receives 360 million gallons of treated sewage discharge from the city of Boston every day, we can assume here that sewage is the dominant input. Now, can you think of any removal processes (that is, outputs) besides water leaving the bay? Pause the video here and write down a couple.

There are many possible outputs, including the rates of dilution, sedimentation, biodegradation, loss to the atmosphere, and photodegradation.

Observe that some of these estrogen outputs remove estrogens from the control volume, while others chemically transform estrogens into other compounds.

At this point we may decide to neglect terms that we suspect will be small given what we know about the characteristics of the particular chemical and environment that we're modeling.

For example, we might neglect loss to the atmosphere because estrogen's structure means it has a low vapor pressure. In addition, the fact that sewage is discharged from a pipe at the seafloor and will be trapped below the sunlit surface allows us to neglect photodegradation. We include the inputs and outputs into the differential equation like so. We're going to make two more simplifying assumptions to make this equation easier to solve. Remember, the goal is not to have a perfect model of estrogens in the bay, but to make a quick computation to estimate how much water I should collect before I will have levels of estrogen that I can detect.

The two simplifying assumptions we make are that: 1. The distribution of estrogens in the control volume is uniform. That is, the bay is "well mixed. 2. The concentration is constant in time, that is the inputs and outputs are balanced. We could solve this equation without assuming that the concentration is constant in time, but this would make our solution a lot more complex, so for OUR back of the envelope calculation, this is OK.

Let's look at the terms in our differential equation. The input rate is represented by the mass flux, which is the mass per time, Q, of estrogen leaving the wastewater treatment plant, divided by the volume, V, of the bay.

Dilution rate is represented by the dilution rate constant K dilution times C.

Sedimentation rate is determined in terms of the concentration of estrogens that are attached to solid particles, since only the estrogen on solid particles will sink.

Keep in mind that the solid particle estrogens are represented by some fraction fs of the total concentration.

So the sedimentation rate is represented by the sedimentation rate constant, k_sed, times the fraction of the concentration of estrogen attached to solid particles.

Biodegradation rate is represented by the biodegradation rate constant k_deg times C.

Assuming steady state we get this equation. Grouping like terms, and solving for C we get this. Now we can isolate C and solve the equation using what we know or can estimate about the chemical or the system.

Once we solved for the concentration of estrogen in the bay, we determined that we needed to collect 20 liters of water in order to make the necessary measurements.

Here you see me on Massachusetts bay collecting water samples.

We would collect 8 samples of 20L of water per day, extract and concentrate each sample down to 100 micro liters before high enough levels of estrogens could be experimentally measured using a mass spectrometer. The model was key in helping me plan my sampling strategy.

It turns out that this quick estimate was pretty good, and I've collected and was able to detect estrogens in

Massachusetts bay.

Now I can use these measurements to refine my model. For example, I might remove the assumption that the concentration is unchanging in time.

By comparing measured and predicted concentrations, we can also hypothesize about which processes are dominant and discover potential missing processes that affect estrogen concentration in the bay. Once these hypotheses are well formed, we can then design new experiments to test them. And can continue to refine the model.

Ultimately, it's the iterative process of taking measurements and refining our model that allows us to answer important questions about whether estrogen levels are likely to pose a hazard in the bay.

We have demonstrated how differential equations and simplifying assumptions can be used to help us predict the concentration of a contaminant in a coastal bay. We have shown a simple example, but the approach can be applied to any chemical in any control volume and at any scale. So, the next time you are marveling at the complexity of the world around you, you can imagine how you might construct a model using differential equations to help you understand it better.