

Ecological modelling Exercises questions

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QUESTIONS

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Exercise 1 Conceptual model – lake eutrophication

Phosphorus is the nutrient that is generally limiting primary production in lakes. Increasing the input of phosphorus increases the concentration of phytoplankton, which may have a radical effect on water quality. Cladoceran grazers (zooplankton) are the main consumers of lake algae and may reduce algal biomass.

To overcome the negative impacts of eutrophication, the concept of biomanipulation was introduced in the seventies, which consisted of reducing the predation pressure on these large cladocerans. When successful, this treatment resulted in a reduced phytoplankton biomass and a higher zooplankton biomass dominated by large Daphnia. However, several cases were reported where this manipulation failed to give the desired results. Close examination revealed that failure was most likely in lakes that received a phosphorus input above a certain critical level.

Tasks:

Make a conceptual model that may serve to investigate the effect of biomanipulation on a lake ecosystem.

Review the components that should be included in the model.

What state variables will be in your model?

What forcings?

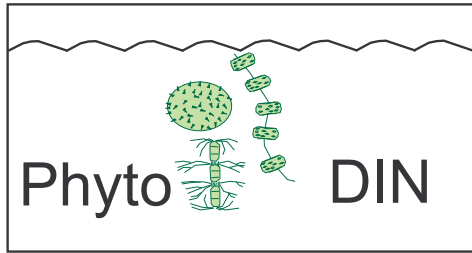
What types of relations?

What will be the space and time scale of your model?

Draw your model structure on a transparency. Some of you will be invited to present it to the group for discussion.

How would you investigate the effect of biomanipulation ?

Exercise 2 Model formulation: nutrient-limited batch culture.



Phytoplankton is grown in a well-mixed culture vessel. At the start of the experiment, the algal concentration is $0.1 \text{ mmol N m}^{-3}$, the dissolved inorganic nitrogen (DIN) concentration 10 mmol N m^{-3} . Other nutrients and light are never limiting the growth of the algae.

We assume:

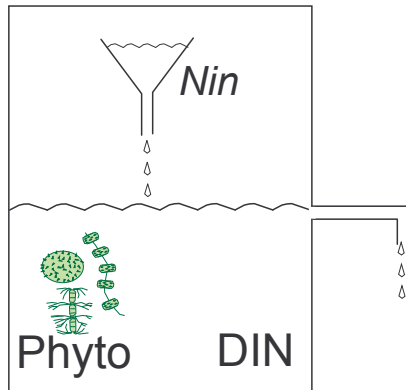
1. The maximum DIN uptake rate of the algae is set by the prevailing light conditions, and given by the parameter **pmax** = 1.0 d^{-1} .
2. Actual nitrogen uptake is governed by Monod kinetics with parameter **ks** = $1.0 \text{ } \mu\text{mol N} \cdot \text{dm}^{-3}$.

$$\text{DINuptakeRate} = p \max \cdot \frac{\text{DIN}}{\text{DIN} + ks}$$

Tasks:

1. What are the units of DINuptakeRate.
2. Investigate the Monod kinetics in a spreadsheet.
 - Make a block with parameters of the model (pmax; ks). Use the Insert/ Names/ create command to give the parameters easy names that can be used in the formulas.
 - Below this block, write the functional dependency in successive columns. In the first column, give a range of DIN, from 0 to $50 \text{ } \mu\text{mol N} \cdot \text{dm}^{-3}$, each value $0.5 \text{ } \mu\text{mol N} \cdot \text{dm}^{-3}$ larger than the previous value. In the next column calculate the DIN uptake rate realised by the algae under these DIN concentrations. Use the named parameters in the equations.
 - Make a graph of this rate as a function of DIN. Now vary the input parameters pmax and ks and look at the consequences for the uptake rate.
3. Make a model that describes the concentration of the algae as a function of time.
 - a. Start with a conceptual model. What are the state variables in this model? Which are the flows? Draw the flow chart.
 - b. Now write the mathematical equations for this model.
4. Check the mass balance of your model. Is mass conserved by your equations?

Exercise 3 Model formulation: nutrient-limited chemostat model



The next experiment that we will model is similar to the previous, except that the culture vessel is not closed.

Now culture medium is pumped continuously into the vessel, where it is mixed homogeneously with the existing contents. An identical amount of the existing contents in the vessel is removed by this process.

We deal with a nutrient-limited chemostat where the culture medium that is pumped into the chemostat is poor in nutrients. Here we will again consider a case with nitrogen limitation, where light is assumed to be

present in surplus.

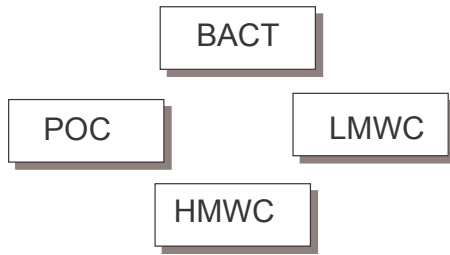
Assumptions:

1. The maximum growth rate of the algae is set by the prevailing light conditions, and given by the parameter **pmax**=1.0 d⁻¹.
2. Nitrogen uptake is governed by Monod kinetics with parameter **ks**=1.0 μmol.dm⁻³.
3. For the concentration of inflowing nitrogen use parameter **Nin**=10 μmol.dm⁻³ and for dilution rate **DilRate** assume that 1% of the vessel content is replaced per hour.

Tasks:

1. Write the coupled model equations.
2. Check the dimensional consistency of your model. Write out the dimensions at both sides of the equality signs and check whether they are the same.
3. Check the mass balance of your model.
Is total mass in the culture vessel always constant? Tip: mass is constant when the rate of change = 0. In this case the rate of change of total nitrogen concentration in the model should be 0. Remember that $d(a+b)/dt = da/dt + db/dt$. Can you find the conditions when total mass in the medium will be constant?
Is mass conserved by your equations? The principle is to compare the rate of change of total nitrogen per unit time in your model with the mass of nitrogen flowing per unit of time over the incoming and outgoing boundaries. All biological terms should cancel in the rate of change of total nitrogen.
4. Investigate the growth rate of the algae as a function of prevailing nutrient concentrations in the medium. Make a column with varying nutrient concentrations. In the next column express DIN uptake rate of the algae as a function of nutrient levels, and in the next express net growth rate (taking into account the parameter **DilRate**). Vary the level of input concentration of nutrients and of dilution rate and look at the changes in growth rate of the algae.

Exercise 4 Detritus-bacteria model



Detritus in the marine system is degraded by the action of heterotrophic bacteria. This is not a one-step process: bacteria cannot 'eat' detritus! You will make a model that is closer to the reality of the process.

It considers that particulate detritus (POC) is first degraded by the action of bacterial exoenzymes to high-molecular-weight dissolved organic carbon (HMWC). This in turn is attacked by enzymes to yield low-molecular-weight dissolved organic carbon (LMWC), which can then be taken up by the bacteria (BACT) which grow on it.

Assumptions:

1. We will not model the exoenzyme concentration explicitly in the model. Instead, we will assume that the maximal rate of hydrolysis (degradation) of POC and of HMWC is proportional to bacterial biomass [note: it are the bacteria that perform the work, they set the maximal rate]. We will use the parameters $K_{\max\text{POC}}$ and $K_{\max\text{HMWC}}$ as maximal specific rates for the hydrolysis of POC and HMWC respectively.
2. The hydrolysis of POC and HMWC is limited by the concentration of the resource. We will use Monod kinetics for both limitations, with half-saturation constants k_{spoc} and k_{shmwC} respectively.
3. POC is produced by algae which are external to our model. We impose a constant influx of POC into the model system as Flux_{POC} . POC is consumed by hydrolysis to HMWC.
4. HMWC is produced by the hydrolysis of POC, and lost by hydrolysis to LMWC.
5. LMWC is produced by the hydrolysis of HMWC, and lost by the uptake by bacteria. Again we assume that maximum uptake is directly proportional to bacterial biomass, with rate parameter U_{\max} , and limited by substrate availability: Monod kinetics with parameter k_{sup} .
6. Bacteria grow by uptake of LMWC, but loose carbon by basal respiration (r_{bas}) and by activity respiration: they respire a fraction p_{loss} of the uptake. Moreover, bacteria are subject to predation, and this is modelled as a quadratic closure term, with parameter r_{clos} .

Summary of parameters and their values:

Model parameters		
$k_{\max\text{poc}}$	0.75	d^{-1}
$k_{\max\text{hmwc}}$	0.5	d^{-1}
U_{\max}	2	d^{-1}
K_{spoc}	100	mmolC.m^{-3}
k_{shmwC}	5	mmolC.m^{-3}
K_{sup}	0.5	mmolC.m^{-3}
R_{bas}	0.1	d^{-1}
p_{loss}	0.5	-
R_{clos}	0.05	$(\text{mmolC.m}^{-3})^{-1}.\text{d}^{-1}$

Forcing function		
FluxPOC	0.5	mmolC.m ⁻³ .d ⁻¹

Tasks :

1. Make a coupled model of this process. First define your state variables. Then for each state variable sketch the influxes and outfluxes in a flow chart. Then write the formulations for each of these fluxes. Finally assemble the differential equations of your state variables as the sums of these positive and negative fluxes.
2. Check the dimensionality of your model.
3. Study the numerical solution of the model that we have prepared in a spreadsheet (bacteria.xls). We used the following initial conditions:

Initial conditions	
POC_init	1000 mmolC.m ⁻³
HMWC_init	5 mmolC.m ⁻³
LMWC_init	0.15 mmolC.m ⁻³
BACT_init	5 mmolC.m ⁻³

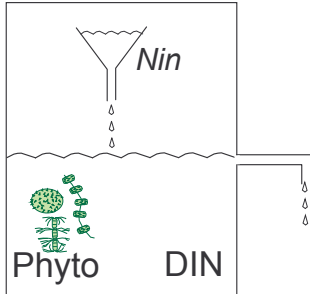
The model is solved numerically using Euler integration:

$$C^{t+\Delta t} = C^t + \Delta t \cdot \frac{dC^t}{dt}$$

A time step Δt (delt in the spreadsheet) of 0.1 d is used.

After a block with parameters, you will find the actual model solution in a number of columns. In a first column, time is updated. The first row has the value time=0, subsequent rows update the value of time by summing the time step Δt to the previous value. The next column is the rate of change of POC. All rows contain the same equation, expressing the rate of change $d\text{POC}/dt$ as a function of the variables and parameters. The next column contains the integrated values of POC. The first row contains the initial value. Subsequent rows update their value by summing $(d\text{POC}/dt) \cdot \Delta t$ to the previous value. The following columns for the other state variables follow exactly the same principle.

Exercise 5 Numerical solution of the nutrient-algae chemostat model



Solve the nutrient-algae chemostat model of example 3 numerically in a spreadsheet.

The model equations:

$$\frac{dPHYTO}{dt} = p \max \cdot \frac{DIN}{DIN + ks} \cdot PHYTO - Dilrate \cdot PHYTO$$

$$\frac{dDIN}{dt} = -p \max \cdot \frac{DIN}{DIN + ks} \cdot PHYTO - Dilrate \cdot (DIN - Nin)$$

with the following parameter values:

pMax	1.0 d ⁻¹
ks	1 mmol N m ⁻³
Nin	10 mmol N m ⁻³
DilRate	0.24 d ⁻¹

And the initial conditions:

DIN(t0)	0.1 mmol N m ⁻³
PHYTO(t0)	1 mmol N m ⁻³

The model is solved numerically using Euler integration:

$$C^{t+\Delta t} = C^t + \Delta t \cdot \frac{dC^t}{dt}$$

Tasks:

1. Simulate the dynamics of phytoplankton – DIN for 20 days.

Make a block with the parameters of the model, and the parameters needed for numerical model solution (initial conditions, timestep Δt). Use the Insert/Names/Create command to give them easy names, so that you can refer to them in your formulas by name. Use 0.1 day as the time step.

Then for $t=0$ make a row of values that contains the following calculations: the actual time t (start with zero), the rate of change of DIN (calculated from the model and its parameters), the actual DIN concentration (start with initial values), the rate of change of algae, the actual algal concentration (initial value). Also calculate the total nitrogen concentration in the model, both as dissolved nutrient and in the algae (sum of nutrient concentration and algal concentration).

Update time and concentrations in the next line. Make use of the following relations (Euler integration):

$$T_i = T_{i-1} + \Delta t$$

$$N_i = N_{i-1} + \Delta t \cdot \frac{dN}{dt}|_{i-1}$$

$$A_i = A_{i-1} + \Delta t \cdot \frac{dA}{dt}|_{i-1}$$

Where the subscript i denotes concentration or rate of change determined at time step i . Actual time is equal to previous time plus time step. Actual nutrient concentration is previous nutrient concentration plus rate of change (calculated in the previous line) * time step. Actual algal concentration is calculated similarly.

Also update the rates of change, by recalculating them on the basis of the new actual concentrations.

Copy this line a number of times down, until a total simulation period of twenty days has been reached.

- a. Make a plot of nutrient and algal concentrations versus time.
- b. Make a plot of algae versus nutrients (phase-plane plot).

2. Change the time step of the model solution.

First decrease it, making sure you have sufficient calculation lines to always simulate a 20-day period. Then increase it in steps of 0.1 d.

What happens to your model solution when you decrease and increase the time step?

3. Set the time step back to 0.1. Now increase p_{\max} from its 'standard' value of 1 d^{-1} in steps of 0.5 d^{-1} .

Watch the stability of your solution. Conclude about the relation between time step length and dynamic properties of the model.

4. Equilibrium points.

Choose an economic and accurate time step based on your previous experience. Now use your model solution scheme to solve the model for a number of initial conditions that are dispersed over the phase plane (with DIN_0 varying from 0 to 5; Algae_0 from 0 to 15). Save your solutions somewhere, and plot the trajectories (Algae versus DIN), starting from different initial conditions, in the phase plane. Conclude about the stability of the equilibrium point(s).

Try different initial conditions that vary from very near to the equilibrium, to very far away from it. How long does it take before the solution for the algae is within 1% of the equilibrium solution? What is the relation between initial conditions and time needed to reach the equilibrium?

Exercise 6 Advection-reaction model

Consider the aphotic part of an oceanic water column (i.e. the part below the euphotic zone). The depth of this column is 400 m. Organic matter is raining down from the productive euphotic zone. As it sinks through the water column, it is being degraded.

Assumptions:

1. The organic matter has a constant sinking velocity v of 50 m.d^{-1} . The sinking of the organic matter is an advective process.
2. We model the degradation as a first-order process, with a degradation rate k of 0.2 d^{-1} .
3. The flux of organic matter from the euphotic zone, i.e. the upper boundary for our model, is prescribed as $\text{Flux} = 100 \text{ mmolC.m}^{-2}.\text{d}^{-1}$. At the lower end of the water column, material leaves the water column to settle on the bottom.
4. We consider no diffusive mixing.

Tasks:

1. Write the model expressing the rate of change of organic matter as an advective-reaction equation.
2. Check the dimensionality of your model. Do dimensions at both sides correspond?
3. Now proceed to solve your model numerically
In a spreadsheet, make a block of parameters. Add the time step and the depth step as additional parameters – you will need them for your solution. As before, use the Insert/Names/Create command to give them easy names, so that you can refer to them in your formulas by name.

Make a column of depths, taking a depth step of 10 m and representing the middle of your boxes (i.e. start at depth 5, then 15 etc.). The last box has depth 395 m.

In the next column give initial values to the concentration of organic matter. We assume the water column is empty, so we take 0 in each box.

In the next column, calculate the depth profile one time step later.
You will have to discretise both time and space for this. As before, use Euler integration to integrate in time:

$$C^{t+\Delta t} = C^t + \Delta t \cdot \frac{dC^t}{dt}$$

use backward differences for your advective term:

$$v \cdot \frac{\partial C}{\partial x} \approx v \cdot \frac{C_x - C_{x-\Delta x}}{\Delta x}$$

You will have to use a different expression for the upper layer than for the other layers. The upper layer must take into account the flux boundary condition, since it cannot know the concentration outside the model domain. Remember that the advective term is a difference of (advective) fluxes at the upper and lower boundary of the cell. Therefore at the upper cell, the advective term will be the difference between the incoming flux (**Flux**) and the outgoing flux ($v \cdot C_1$), divided by the thickness of the box [where **Flux** is the imposed boundary flux, and C_1 is the concentration in the upper compartment].

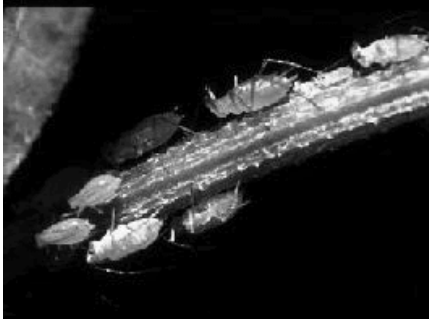
For all following compartments, the advective term will be a function of the concentrations in the boxes.

Then copy this column a number of times to the right, and make sure there is also a row that updates time. Look in a figure how your depth profile of organic matter is evolving in time. Spreadsheets are not very suitable for this kind of calculations. However, you may get an idea of how the numerical solution of this type of equations works.

4. The analytical solution.

It is relatively easy, in this case, to calculate the steady state analytically. Put the rate of change in time equal to zero, and solve the resulting differential equation in x by integration (if you have some time left). The solution is very similar to the solution of the exponential growth equation that was discussed in the lecture. Compare the analytical solution for the steady state with the result of your spreadsheet solution after you have reached steady state in the spreadsheet.

Exercise 7 Diffusion-reaction model



Consider a row of plants, 60 m long. In the middle of the row, a small population of aphids invades the plants.

Assumptions:

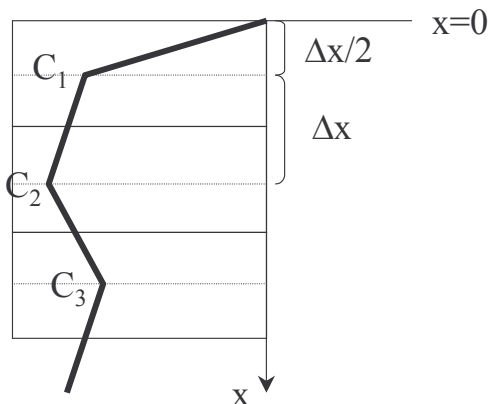
The aphids reproduce with a net rate of increase $r=0.01 \text{ d}^{-1}$. Note this is a very low value, but it is a *net* rate of increase, i.e. difference between birth and mortality processes, and we assume that the plants are not very good food, so that the aphids just barely survive.

The aphids slowly disperse from their original location. This dispersal is by random movement, and can be modelled as a diffusion process with diffusion coefficient $K=0.3 \text{ m}^2\text{d}^{-1}$. At both ends of the row of plants, aphids that happen to move outside will disappear forever. Therefore we can set as spatial boundary conditions that concentrations are zero outside the model domain, i.e. at $x=0\text{m}$ and $x=60\text{m}$.

Tasks:

1. Construct a diffusion-reaction model for the process. Check the dimensions.
2. Solve your model numerically in a spreadsheet. Organise your spreadsheet as in previous Exercise. Use a spatial step of 1 m, and a time step of 1 d. Use spatial discretisation for second-order equations as specified in the lecture notes and reproduced here:

$$\begin{aligned} \frac{\partial}{\partial x} \left[K \cdot \frac{\partial C}{\partial x} \right] &= \frac{[K \cdot \frac{\partial C}{\partial x}]_{i+1/2} - [K \cdot \frac{\partial C}{\partial x}]_{i-1/2}}{\Delta x} \\ &= \frac{K \cdot \frac{C_{i+1} - C_i}{\Delta x} - K \cdot \frac{C_i - C_{i-1}}{\Delta x}}{\Delta x} \\ &= \frac{K \cdot (C_{i+1} + C_{i-1} - 2C_i)}{\Delta x^2} \end{aligned}$$



At the boundaries, special care is needed. The value right at the boundary ($x=0$, $x=60$) should be zero, and since we model concentrations in the middle of the cells (i.e. at 0.5 m, 1.5 m .. 59.5 m), we have to make sure that our calculations reflect the boundary values $C=0$ at $x=0$ and $x=60$. It is best to consider the diffusive process as a gradient of fluxes, as in the middle formula above: the difference between outgoing flux $[-K \cdot (C_{i+1} - C_i) / \Delta x]$ and the incoming flux $[-K \cdot (C_i - C_{i-1}) / \Delta x]$, divided by Δx . Remember that for diffusive processes, the flux is the negative of the diffusion

coefficient times the concentration gradient. At the upper boundary, we have no value for C_{i-1} , as if falls outside the model domain. However, it *is* possible to estimate the concentration gradient there, and thus the incoming flux. Consider the scheme:

It is easy to see that the concentration gradient between the first and the second box can be approximated as $(C_2 - C_1) / \Delta x$. Likewise, one can see that the concentration gradient at the upper boundary of the upper box is given as $C_1 / (\Delta x / 2)$, or $2C_1 / \Delta x$. This value can then be plugged into the equation for the diffusion flux.

For the lower boundary, the reasoning is exactly the same.

Summary of model parameters and constants needed for solution:

Parameters		
r	0.01	d ⁻¹
D	0.3	m ² .d ⁻¹
Solution constants:		
Delt	1	d
Delx	1	m

Initial conditions: make the density 0 everywhere, except at the cells with middle point 29.5 and 30.5, where the initial density is 1.

Exercise 8 An analytical model of oxygen in the sediment.

Consider the dynamics of oxygen in a marine sediment in the absence of primary production. Oxygen is exchanged by molecular diffusion and sediment advection and is consumed by a variety of processes that relate to organic matter degradation. We will analyse a simple model that describes oxygen consumption in the sediment and the resulting depth profile.

Assumptions.

The sediment oxygen profile has reached steady-state
Oxygen is consumed at a first-order rate.

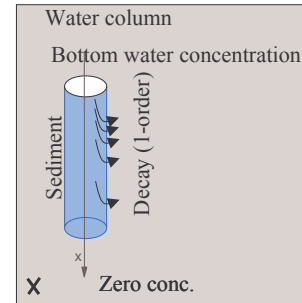
The model is given by the advection-diffusion-reaction equation:

$$\frac{\partial C}{\partial t} = 0 = D \frac{\partial^2 C}{\partial x^2} - w \frac{\partial C}{\partial x} - kC$$

At the sediment-water interface the concentration of oxygen in the overlying water is specified. Oxygen consumption in the sediment proceeds until all oxygen is exhausted. The boundary conditions then read:

$$C_{x=0} = C_0$$

$$C_{x=\infty} = 0$$



Tasks:

- Find the particular solution that describes the oxygen concentration as a function of sediment depth. (compare with the analytical solution of carbon dynamics in lecture notes, page 48).
- Implement the analytical solution in a spreadsheet. Use k , D , w and C_0 as parameters, and solve the equation for $x=0, 0.1, 0.2, \dots 50$ mm depth. The following parameter values are given; they are typical for continental slope sediments:

K	10	d ⁻¹
D	1.10 ⁻⁵	cm ² s ⁻¹
W	1	mm yr ⁻¹
C ₀	300	mmol m ⁻³

Make a graph of oxygen concentration versus sediment depth.

- SENSITIVITY: Increase and decrease k and w by one to two orders of magnitude (abyssal to coastal sediments). Investigate the consequences for oxygen. For each of these cases, calculate the flux of oxygen in the sediment; calculate the flux analytically. Recall that:

$$Flux = -D \frac{\partial C}{\partial x} + wC_{x=0}$$

and that

$$\frac{\partial e^{ax}}{\partial x} = a \cdot e^{ax}$$

Which is the most sensitive parameter ?

4. SENSITIVITY: Calculate analytically the oxygen penetration depth (= depth where oxygen=1 mmol.m⁻³) as a function of oxygen flux for varying values of k. Make a graph of oxygen penetration versus oxygen flux, expressed in mmol m⁻² d⁻¹
5. CALIBRATION. Assume the following measurements have been performed, using micro-electrodes:

Depth cm	O ₂ conc mmol m ⁻³
0	300.00
0.1	65.52
0.2	14.31
0.3	3.13
0.4	0.68
0.5	0.59
1	0.27

Estimate the values of the parameters that can explain these observations. Which parameter would you vary in the first place? You may limit your search for optimal parameter values to this most sensitive parameter. Try different values and compare the model result with the observations.

As an alternative, you may use the Excel solver function for the estimation of optimal parameter values. We will show you how to do this. It is a powerful method for estimation in problems that are not too complex.

Question: what is the flux of oxygen across the sediment-water interface?