

# Ecological modelling Exercises Answers

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## **ANSWERS**

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## Exercise 1 Conceptual model of lake eutrophication - Solution

A minimal model of a lake ecosystem should at least describe dissolved inorganic P (DIP), algae and zooplankton. These are all state variables. We might also consider the inclusion of fishes, but these are generally more difficult to model. A good alternative is to mimic the effect of fishes on the zooplankton through a mortality coefficient.

The processes of primary production, phytoplankton grazing by zooplankton, excretion and mortality will be included.

It is always best to start with a simple model, Here we will assume that the water is well mixed, such that the spatial scale will be the entire lake. A typical time scale is the seasonal cycle.

Lakes are generally open, flow-through systems, where water and nutrients are supplied through the inflows and lost through the outflows. The water flow and nutrient input INTO the lake depends on external conditions (processes that occur in the inflowing river, i.e. outside the control of the model). If these inputs change a lot over time, we will impose them as forcing functions in the model. If they are roughly constant, we could use a parameter instead.

As the lake is well mixed, the concentration of DIP, algae and zooplankton in the outflowing water will equal the concentration in the lake. We will assume that the lake volume does not change, so the flow rate of water out of the lake equals the inflow rate. By doing so, we do not need additional parameters or forcing functions to represent outflow.

If primary production is also light limited at certain times, we also need solar radiation, a forcing function.

Summarising:

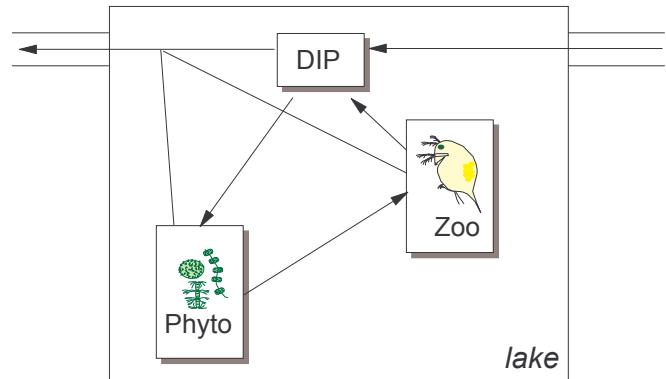
State variables:

- Dissolved inorganic P (DIP),
- Phytoplankton,
- Zooplankton

Forcing functions:

- Flow rate into the lake and DIP concentration in inflowing water
- Solar radiation

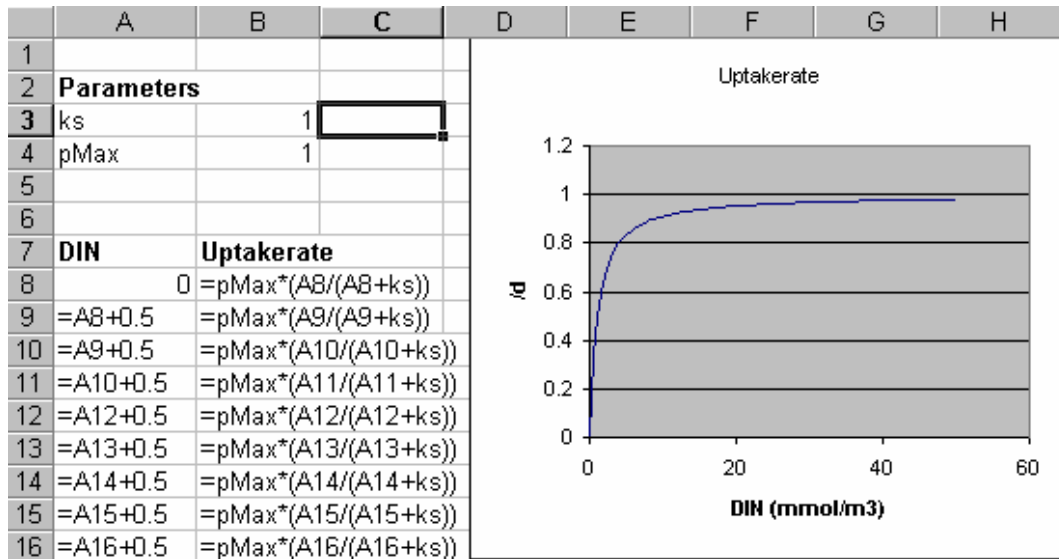
The effect of biomanipulation could be investigated by changing the zooplankton mortality under different flowrate regimes.



## Exercise 2 Formulating the nutrient-limited batch culture model - Solution



1. With  $p_{max}$  in  $d^{-1}$ , the units of  $DIN_{uptake}$  are also  $d^{-1}$ .
2. The units of  $k_s$  are  $\mu\text{mol N}\cdot\text{dm}^{-3}$  or  $\text{mmol N m}^{-3}$ . The spreadsheet that investigates the Monod kinetics might look like this:



Varying the value of  $p_{max}$  changes the asymptotic (maximal) value of the uptake rate.  $K_s$  is the 'half-saturation' constant, i.e. the concentration of DIN at which the uptake rate is half its maximal value. Changing its value changes the shape of the functional dependency.

3. Although we only want to know how the algae change as a function of time, it is necessary to consider both nutrients and algae in a coupled model. This is because the availability of DIN determines the uptake rate of the algae. The conceptual model comprises two state variables: the concentration of algae (Phyto,  $\text{mmol N m}^{-3}$ ) and of DIN ( $\text{mmol N m}^{-3}$ ). The uptake of DIN by the algae is a source to the algae and a sink for the nutrients. Total DIN uptake rate ( $\text{mmol N m}^{-3} d^{-1}$ ) takes into account the concentration of the algae. (the higher algal concentration, the higher the nitrogen uptake rate)

$$\frac{dPhyto}{dt} = pMax \cdot \frac{DIN}{DIN + ks} \cdot Phyto$$

$$\frac{dDIN}{dt} = -pMax \cdot \frac{DIN}{DIN + ks} \cdot Phyto$$

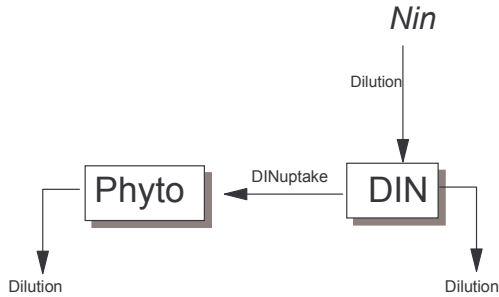
The units of  $dPhyto/dt$  are  $\text{mmol N m}^{-3} d^{-1}$

The model is fully specified if we also provide the initial conditions:

$$\begin{aligned}\text{Phyto}(t_0) &= 0.1 \text{ mmol N m}^{-3} \\ \text{DIN}(t_0) &= 10.0 \text{ mmol N m}^{-3}\end{aligned}$$

4. Mass is fully conserved: the amount of mass that leaves DIN enters the Phytoplankton.

## Exercise 3 Formulating the nutrient-limited chemostat model - Solution



1. In addition to the previous exercise, the medium is diluted at a constant rate of  $1\% \text{ hour}^{-1}$ .

With all the other parameters in days, we need to recalculate the dilution rate in  $\text{d}^{-1}$ .  $0.01 \text{ hr}^{-1}$  is equivalent to  $0.24 \text{ d}^{-1}$ . (you will dilute 24 times more volume in one day compared to one hour).

Diluting effectively replaces vessel medium (which consists of DIN and

PHYTO) by culture medium with known concentration  $N_{in}$ . It is a sink to PHYTO in the vessel, it replaces a certain amount of DIN in the vessel by  $N_{in}$ .

The coupled model is given by the following equations:

$$\frac{d\text{Phyto}}{dt} = p_{\max} \cdot \text{Phyto} \cdot \frac{\text{DIN}}{\text{DIN} + k_s} - \text{Dilrate} \cdot \text{Phyto}$$

$$\frac{d\text{DIN}}{dt} = -p_{\max} \cdot \text{Phyto} \cdot \frac{\text{DIN}}{\text{DIN} + k_s} + \text{Dilrate} \cdot (\text{Nin} - \text{DIN})$$

where **Phyto** is biomass of algae ( $\mu\text{molN} \cdot \text{dm}^{-3}$ ), **DIN** is concentration of dissolved nitrogen ( $\mu\text{molN} \cdot \text{dm}^{-3}$ ), and the parameters are as given in the question.

2. Dimensional check.

For the algal equation, the dimensions are as follows:

$$\frac{d\text{Phyto}}{dt} = p_{\max} \cdot \text{Phyto} \cdot \frac{\text{DIN}}{\text{DIN} + k_s} - \text{Dilrate} \cdot \text{Phyto}$$

$$\frac{\mu \text{ molN} \cdot \text{dm}^{-3}}{\text{d}} = \frac{1}{\text{d}} * \mu \text{ molN} \cdot \text{dm}^{-3} * \frac{\mu \text{ molN} \cdot \text{dm}^{-3}}{\mu \text{ molN} \cdot \text{dm}^{-3} + \mu \text{ molN} \cdot \text{dm}^{-3}} - \frac{1}{\text{d}} * \mu \text{ molN} \cdot \text{dm}^{-3}$$

$$\mu \text{ molN} \cdot \text{dm}^{-3} \cdot \text{d}^{-1} = \mu \text{ molN} \cdot \text{dm}^{-3} \cdot \text{d}^{-1} - \mu \text{ molN} \cdot \text{dm}^{-3} \cdot \text{d}^{-1}$$

which shows the consistency of dimensions. (Note that the dilution rate must be expressed in units  $\text{d}^{-1}$  for this consistency!)

For the nutrients equation the solution is completely analogous.

3. Mass conservation can be tested by writing the rate of change of total nitrogen in the model.

$$\frac{d(\text{Phyto} + \text{DIN})}{dt} = p_{\max} \cdot \text{Phyto} \cdot \frac{\text{DIN}}{\text{DIN} + k_s} - \text{Dilrate} \cdot \text{Phyto} - p_{\max} \cdot \text{Phyto} \cdot \frac{\text{DIN}}{\text{DIN} + k_s} + \text{Dilrate} \cdot (\text{Nin} - \text{DIN})$$

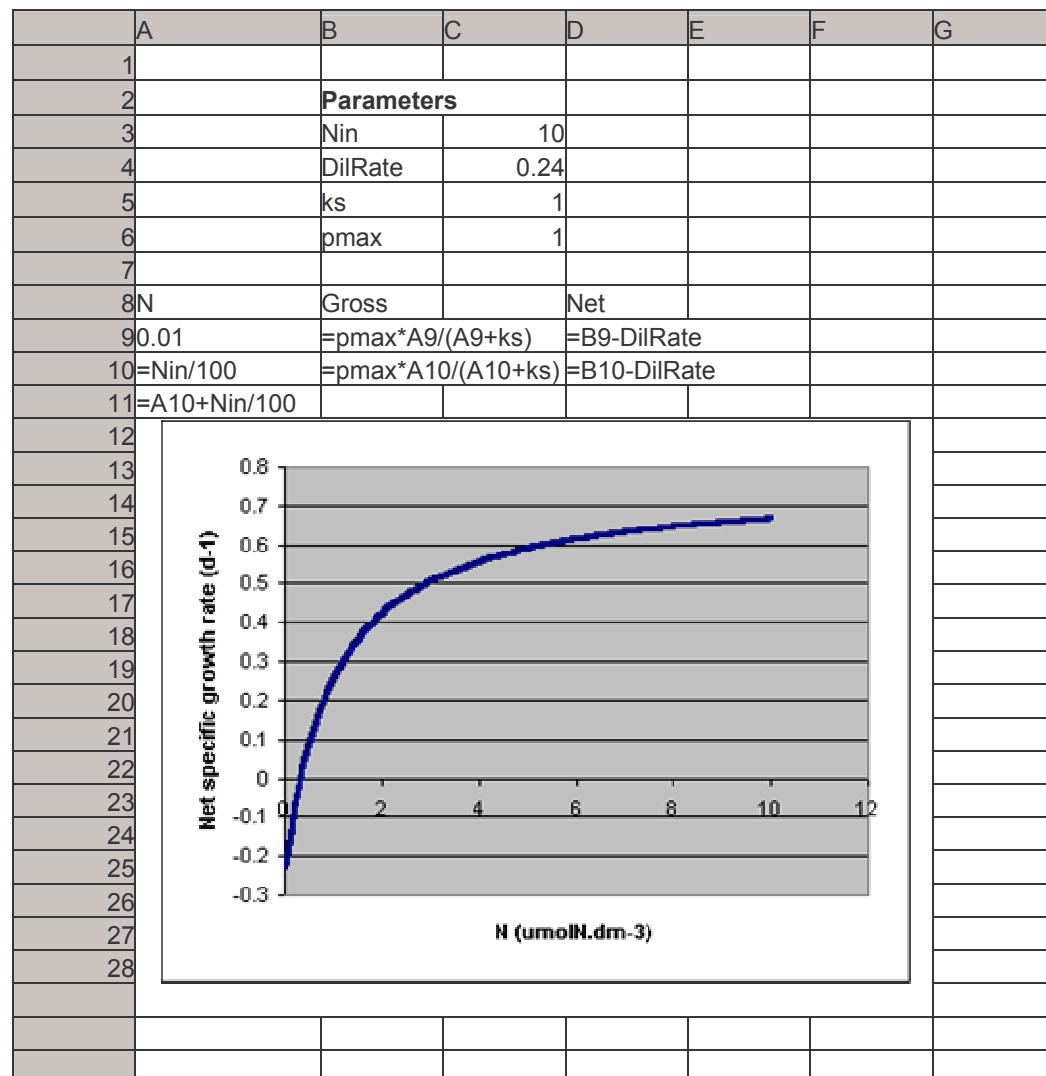
$$= \text{Dilrate} \cdot \text{Nin} - \text{Dilrate} \cdot (\text{Phyto} + \text{DIN})$$

$$= \text{Inflow} - \text{outflow}$$

The total mass in the culture vessel is not necessarily constant. Only when Inflow = Outflow will this be the case. This is when  $N_{in} = \text{Phyto} + \text{DIN}$ , or when the total amount of nitrogen in the culture vessel equals the amount of nitrogen in the culture medium.

For mass to be conserved in the model, the rate of change of total nitrogen must be equal to inflow-outflow. Mass is indeed conserved by the model equations.

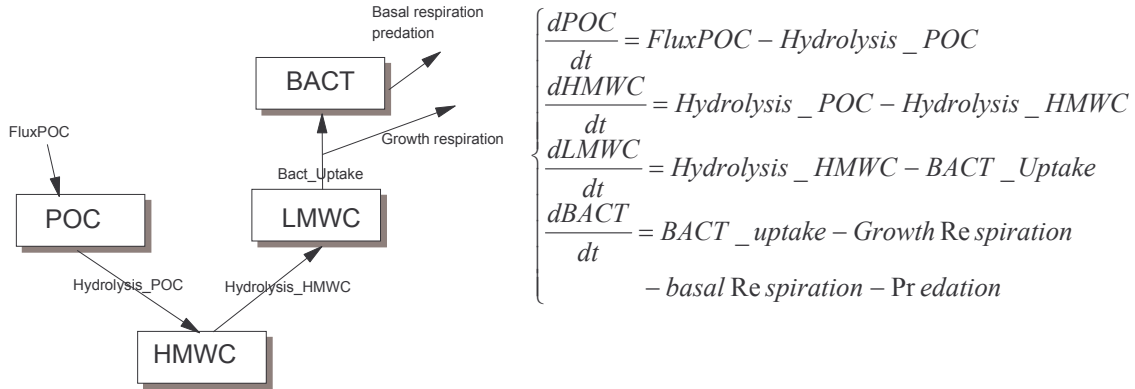
Investigating the growth rate of the algae can be done in a spreadsheet like this:





## Exercise 4 Detritus-bacteria model - Solution

1. We may write the flow chart and conceptual model equations as follows:



The mathematical model equations are:

$$\begin{cases} \frac{dPOC}{dt} = FluxPOC - BACT * k_{max\ poc} * \frac{POC}{POC + k_{spoc}} \\ \frac{dHMWC}{dt} = BACT * k_{max\ poc} * \frac{POC}{POC + k_{spoc}} - BACT * k_{max\ hmw} * \frac{HMWC}{HMWC + k_{shmw}} \\ \frac{dLMWC}{dt} = BACT * k_{max\ hmw} * \frac{HMWC}{HMWC + k_{shmw}} - BACT * UP_{max} * \frac{LMWC}{LMWC + k_{sUp}} \\ \frac{dBACT}{dt} = BACT * UP_{max} * \frac{LMWC}{LMWC + k_{sUp}} * (1 - pLoss) - r_{bas} * BACT - r_{clos} * BACT * BACT \end{cases}$$

3. The solution of the model is in a spreadsheet.

Note: this model is what we call a ‘very stiff’ model, indicating that there are large differences in the rates that together form the model. Such a model usually has to be run for a long time in order to reach steady state, as the steady state is determined by the slowest process in the model (here: hydrolysis of POC). However, it has to be run with a small time step, as the stability of the solution is determined by the fastest process (here: uptake of LMWC by bacteria). Stiff models are a numerical nightmare. There are special algorithms to solve this type of models numerically, and these are much more sophisticated than what we can show here in a spreadsheet !

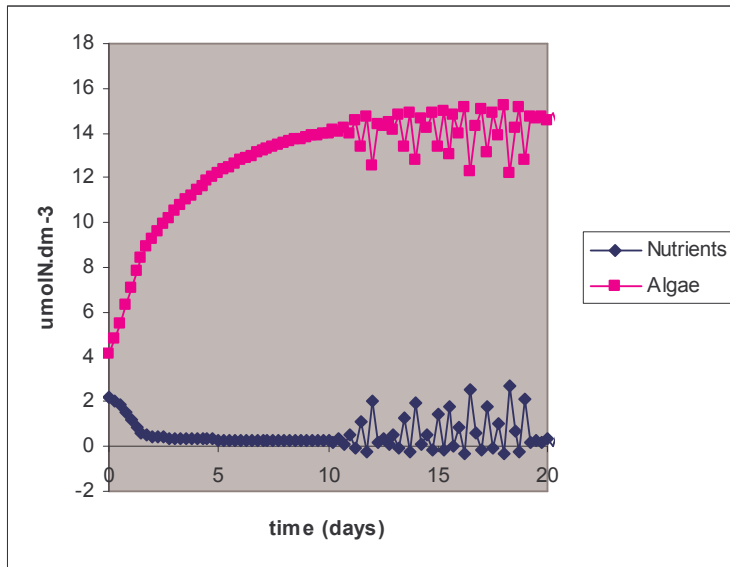
## Exercise 5 Numerical solution of the nutrient-algae chemostat model - Solution

1. Your spreadsheet should look like this:

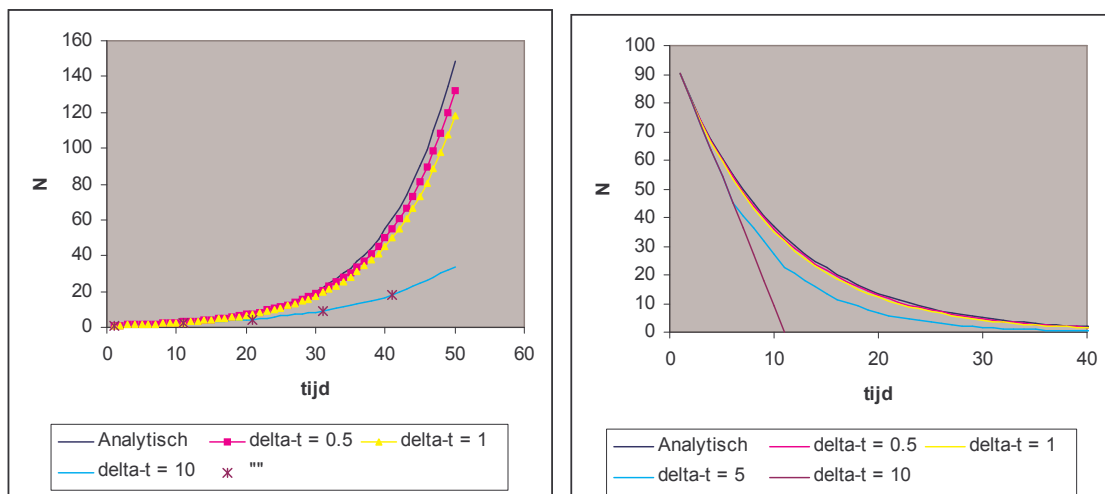
	A	B	C	D	E	F	G
1		<b>Parameters</b>					
2		ks	1				
3		Nin	15				
4		dilrate	0.24				
5		deltat	0.1				
6		Nnul	2.1834172				
7		Anul	4.160943484				
8		pmax	1.237143929				
9							
10	time	dN/dt	N	dA/dt	A	d(totN)/dt	infl-outfl
11		= -E11 * pmax * C11/(ks+C11) + dilrate*Nin- dilrate*C11	=Nnul	=E11 * pmax * D11/(ks+D11) - dilrate*E11	=Anul	=B11+D11	=dilrate*(Nin- C11-E11)
12	=A10+deltat	= -E12 * pmax * C12/(ks+C12) + dilrate*Nin- dilrate*C12	=C11+deltat*B10	=E12 * pmax * D12/(ks+D12) - dilrate*E12	=E11+deltat*D10	=B12+D12	=dilrate*(Nin- C12-E12)
13							
14							
15							
16							
17							
18							
19							
20							
21							
22							
23							
24							
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30							
31							

2. Decreasing the time step should not change your solution very much, although it will become slightly more accurate and will need a lot more lines in the spreadsheet for the same period. When increasing your time step, you will see instabilities appear in the solution. E.g. with the current settings, but deltat=0.25, the first oscillations will appear, as shown in the next figure:



The reason is that the solution becomes increasingly more inaccurate as the time step increases. The rate of change, evaluated at the previous time step, is extrapolated over the entire time step. It is then assumed that the rate of change does not change over this time step. The longer this time step, the larger the error:

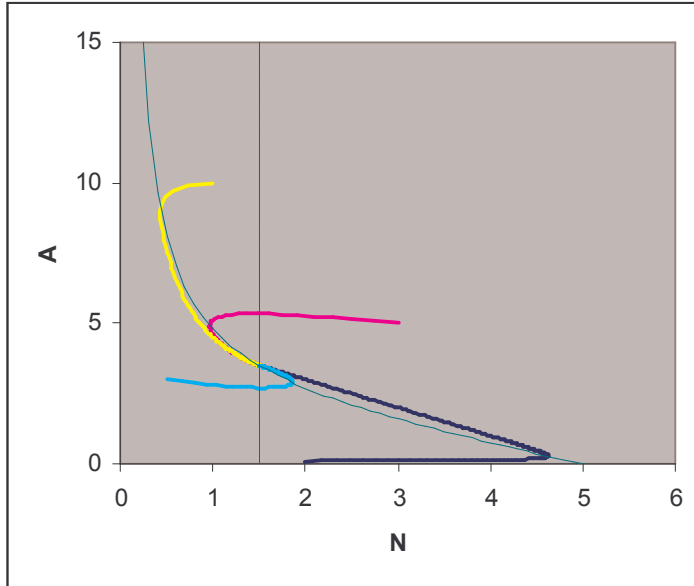


The figures show the approximation by Euler integration of an exponentially increasing and decreasing function with ever increasing time steps. For the negative exponential, a time step of 10 units results in a state variable becoming zero in one time step.

In the case of the chemostat shown above, the nutrient concentration has become negative due to an overshoot error. As mathematical algae grow very well on negative mathematical nutrients, the solution begins to oscillate.

4. Study of model trajectories. Make sure all parameters are set to the same values as used in the first question (using the values in the table). Choose initial values for N and A from one of the sectors of the diagram. The model produces a time plot of N and A. Copy the

columns containing these numbers. Go to a separate worksheet and use 'Paste Special - Values' to paste your results. Repeat for a number of different initial conditions. Plot for each of these series A versus N as different series in the same plot. In the example below we also plotted the isoclines for reference (a straight vertical line, and a curved line). The middle equilibrium point ( $N=1.5$ ,  $A=3.5$ ) is stable. It attracts the trajectories from all starting points in the domain.



The time needed to go to the equilibrium is mainly determined by the initial value of A. If this is very low, it takes a long time for the algae to catch up. For most other initial conditions, except very near to the equilibrium, the time needed does not vary very much.

## Exercise 6 Advection – reaction model. Solution

1. The model equation can be expressed as follows:

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} - k * C$$

where the first part expresses the advection by sinking, and the second part the (first-order) degradation of the organic material.

2. Dimensions:  $\frac{\text{mmolC} \cdot \text{m}^{-3}}{\text{d}} = \text{m} \cdot \text{d}^{-1} \frac{\text{mmolC} \cdot \text{m}^{-3}}{\text{m}} - \text{d}^{-1} \text{mmolC} \cdot \text{m}^{-3}$

These dimensions are consistent, as the **m**'s in numerator and denominator of the first term on the right hand side cancel.

3. The numerical solution of the model is given in the file 'watercolumn.xls' in your marelac directory. Copy or print it. It looks like this:

	A	B	C	D
1				
2	Parameters			
3	k_		0.2	
4	v_		50	
5	Flux		100	
6	Delt		0.1	
7	Delx		10	
8				
9	Time ->		0	0.1 0.2
10	Depth			
11	5		0 =B11+(Flux-V_ V_*B11)/delx- k_*B11)*delt	=C11+(Flux-V_ k_*C11)*delt
12	15		0 =B12+(v_*(B11- B12)/delx-k_*B12)*delt	=C12+(v_*(C11-C12)/delx- k_*C12)*delt
13	25		0 =B13+(v_*(B12- B13)/delx-k_*B13)*delt	=C13+(v_*(C12-C13)/delx- k_*C13)*delt

4. The analytical solution of the steady state goes as follows:

Equalling the rate of change with time to zero, we obtain:

$$0 = -v \frac{dC}{dx} - k * C$$

$$\frac{dC}{dx} = -\frac{k}{v} * C$$

(note that partial derivatives,  $\frac{\partial}{\partial t}$ ,  $\frac{\partial}{\partial x}$  are replaced by ordinary derivatives here,  $\frac{d}{dx}$ , since at steady state the concentration is no longer a function of t, but only of x):

The general solution of this ordinary derivative is given by

$$C = A \exp\left(-\frac{k}{v} x\right)$$

The integration constant A is determined from the upper boundary condition.

For  $x=0$ , we find that the exponent term vanishes (as  $\exp(0) = 1$ ) and  $A=C_0$

$$C_0 = A \exp\left(-\frac{k}{v} 0\right) = A$$

We can calculate the value of  $C_0$  based on the flux that is specified at the upper boundary: we have **Flux**=100 mmol.m<sup>-2</sup>.d<sup>-1</sup>.

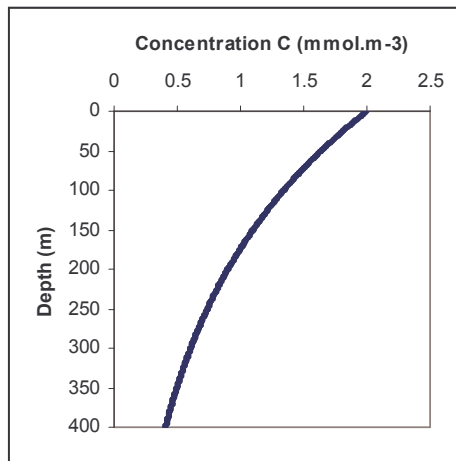
We note that an advective flux is given as  $v \cdot C$ , therefore  $C_0$  (concentration at  $x=0$ ) can be calculated as:

$$C_0 = \text{Flux} / v.$$

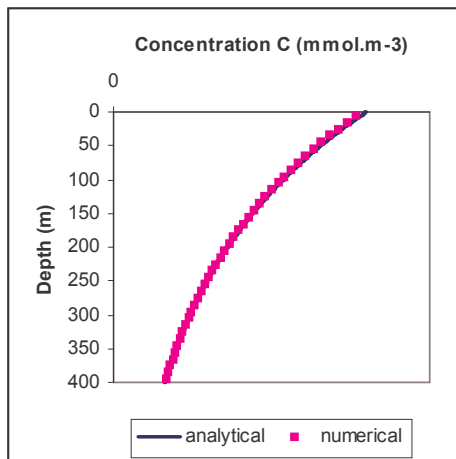
Therefore the particular solution is:

$$C = \frac{\text{Flux}}{v} \exp\left(-\frac{k}{v} x\right)$$

which is shown in the following figure for the parameter values given in the question.



A comparison between analytical and numerical steady state is in the following figure:



## **Exercise 7 Diffusion-reaction model – Solution**

Look up the solutions in the spreadsheet

## Exercise 8 Sediment oxygen model - solution

1. The general solution to the advection-diffusion-reaction equation is found in a book or on page 48 of the lecture notes:

$$C(x) = A \cdot e^{\frac{w - \sqrt{w^2 + 4 \cdot k \cdot D}}{2D} \cdot x} + B \cdot e^{\frac{w + \sqrt{w^2 + 4 \cdot k \cdot D}}{2D} \cdot x}$$

Using the boundary  $C_{x=\infty} = 0$  we derive that  $B = 0$  (similarly as on page 49).

We then paste the upper boundary condition:  $C_{x=0} = C_0$  into the general solution:

$$C_{x=0} = C_0 = A \cdot e^{\frac{w - \sqrt{w^2 + 4 \cdot k \cdot D}}{2D} \cdot 0} = A$$

such that the particular solution can be calculated:

$$C(x) = C_0 \cdot e^{\frac{w - \sqrt{w^2 + 4 \cdot k \cdot D}}{2D} \cdot x}$$

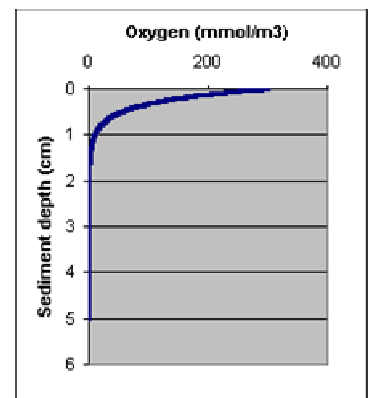
2. In order to implement the analytical solution in a spreadsheet, we have to convert all parameters into common units, e.g. in cm and days.

This means expressing the depth axis in cm, multiplying  $D$  with 86400 and dividing  $w$  by 3650.

The value of  $C_0$  can be used as such, but is expressed in  $\text{nanomol cm}^{-3}$  ( $10^{-9} \text{ mol cm}^{-3}$ ), which is equivalent to  $\text{mmol m}^{-3}$ .

The spreadsheet may look like this:

1	A	B	C	D	E
2	<b>Parameters</b> Common units			Original values	
3	k_	10	d-1	10	d-1
4	D_	=D4*24*60*60	cm2.d-1	0.00001	cm2s-1
5	w_	=D5/10/365	cm.d-1	1	mm.y-1
6	C0	300	nanomol.cm-3	300	mmol.m-3
7					
8	Derived values				
9	a	=(w_-SQRT(w_*w_+4*D_*k_))/(2*D_)			
10	Flux	=-D_*C0*a+w_*C0			
11					
12	depth(cm)	Oxygen			
13	0	=C0*EXP(a*A13)			
14	=0.01+A13	=C0*EXP(a*A14)			
15	=0.01+A14	=C0*EXP(a*A15)			
16	=0.01+A15	=C0*EXP(a*A16)			
17	=0.01+A16	=C0*EXP(a*A17)			





3. Flux is calculated by pasting the analytical solution of C into the flux formula:

$$Flux = -D \frac{\partial C}{\partial x} \bigg|_{x=0} + wC_{x=0} \text{ for depth } x = 0.$$

$$\text{This gives: } Flux = -D \cdot C_0 \cdot \frac{w - \sqrt{w^2 + 4 \cdot k \cdot D}}{2D} + w \cdot C_0.$$

Remark that fluxes are expressed in  $\text{nanomol cm}^{-2} \text{ d}^{-1}$ . To convert to  $\text{mmol m}^{-2} \text{ d}^{-1}$  it has to be divided by 100.

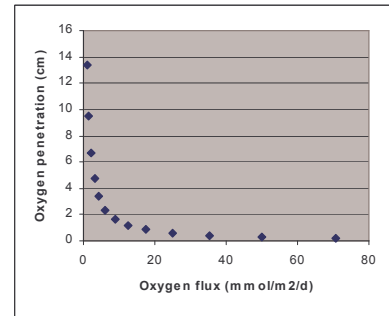
W, the advection rate has almost no effect on the modeled oxygen distribution and the flux. In contrast, changing k has large effect on the oxygen distribution and flux. K is the most sensitive parameter.

4. The oxygen penetration depth can be estimated analytically: it is defined here as the depth where oxygen concentration =  $1 \text{ mmol m}^{-3}$ . We find it by setting:

$$C(x) = C_0 \cdot e^{\frac{w \cdot \sqrt{w^2 + 4 \cdot k \cdot D}}{2D} \cdot x} = 1 \text{ and solving for } x:$$

$$\frac{w \cdot \sqrt{w^2 + 4 \cdot k \cdot D}}{2D} \cdot x_{OX=1} = LN\left(\frac{1}{C_0}\right)$$

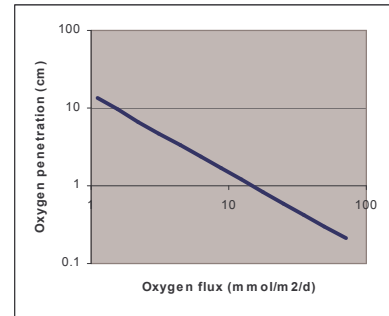
$$x_{OX=1} = LN\left(\frac{1}{C_0}\right) \cdot \frac{2D}{w \cdot \sqrt{w^2 + 4 \cdot k \cdot D}}$$



With increasing fluxes the oxygen penetrates less deep. At first this may seem contra-intuitive. However, oxygen fluxes into the sediment to fulfill the demand of the oxygen consumption processes. This is, at steady-state:

Oxygen flux into the sediment = total oxygen consumption of the sediment.

With increasing oxygen consumption (and hence increasing flux), the amount of oxygen in the sediment decreases, hence the penetration depth decreases.



5. Calibration. The parameters to vary are the ones the model is most sensitive to, i.e. the first-order consumption rate.

The excel solver is a handy tool to find the minimum or maximum of a certain cell by varying a selection of parameters. To apply it for model calibration, you have to minimise the MODEL COST, which is the sum of squared residuals of model values and observations and allow the solver to change the parameter values that must be fine-tuned. Make a table with sediment depth and observed values in two columns and calculate the modeled values at the observed depths, using the analytical formula in a third column. Now calculate in a fourth column, for each observation the squared residual with the model:  $(\text{modeled value} - \text{Observed value})^2$ . Sum all these residuals. This is the model cost, the value that has to be minimized.

Inspect the sheet that performs the model calibration.

To run the solver: select from the menu: tools/solver (you may need to install this feature: tools/add ins).

Set Target cell to \$D\$20, which is the cell containing the model cost. Select the minimum (equal to); set the cell to be changed equal to \$B\$2, which is the cell containing the value of k. Press solve.

The flux of oxygen across the sediment-water interface was 39 mmol m<sup>-2</sup> d<sup>-1</sup>. (K = 200 d<sup>-1</sup>)