

# **Ecosystem Modelling : Introductory course**

## **Exercises**

**Malta, 8 June 2009**

**Exercises from MARELAC  
courses**

# Questions

## 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?

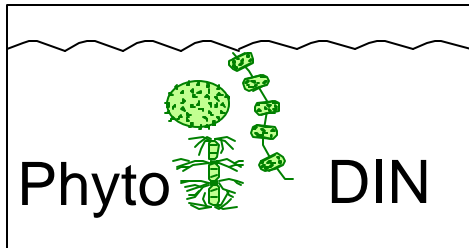
What types of relations?

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  $10 \text{ mmol N m}^{-3}$ . Other nutrients and light are never limiting the growth of the algae.

We assume:

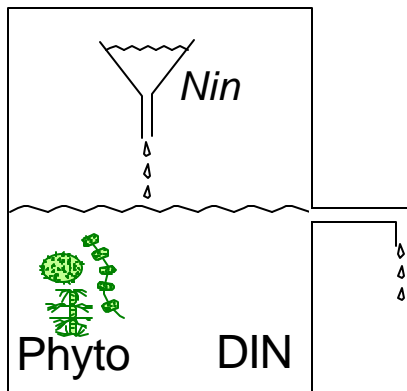
1. The maximum DIN uptake rate of the algae is set by the prevailing light conditions, and given by the parameter  $p_{\max}=1.0 \text{ d}^{-1}$ .
2. Actual nitrogen uptake is governed by Monod kinetics with parameter  $k_s=1.0 \text{ } \mu\text{mol N.dm}^{-3}$ .

$$\text{DINuptakeRate} = p_{\max} \cdot \frac{\text{DIN}}{\text{DIN} + k_s}$$

Tasks:

1. What are the units of DINuptakeRate.
2. Investigate the Monod kinetics in a spreadsheet.
  - Make a block with parameters of the model ( $p_{\max}$ ;  $k_s$ ). 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  $50 \text{ } \mu\text{mol N.dm}^{-3}$ , each value  $0.5 \text{ } \mu\text{mol N.dm}^{-3}$  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  $p_{\max}$  and  $k_s$  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.

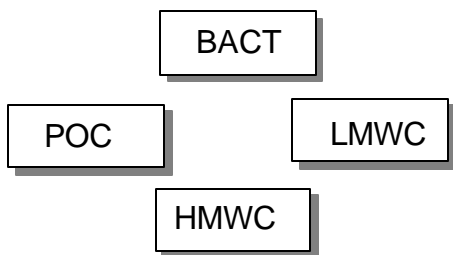
### Assumptions:

1. The maximum growth rate of the algae is set by the prevailing light conditions, and given by the parameter  $\mathbf{pmax}=1.0 \text{ d}^{-1}$ .
2. Nitrogen uptake is governed by Monod kinetics with parameter  $\mathbf{ks}=1.0 \mu\text{mol.dm}^{-3}$ .
3. For the concentration of inflowing nitrogen use parameter  $\mathbf{Nin}=10 \mu\text{mol.dm}^{-3}$  and for dilution rate  $\mathbf{DilRate}$  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  $\mathbf{DilRate}$ ). 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  $ks_{\text{POC}}$  and  $ks_{\text{HMWC}}$  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  $\text{Flux}_{\text{POC}}$ . 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  $UP_{\max}$ , and limited by substrate availability: Monod kinetics with parameter  $ks_{\text{UP}}$ .
6. Bacteria grow by uptake of LMWC, but loose carbon by basal respiration ( $r_{\text{bas}}$ ) and by activity respiration: they respire a fraction  $p_{\text{loss}}$  of the uptake. Moreover, bacteria are subject to predation, and this is modelled as a quadratic closure term, with parameter  $rc_{\text{los}}$ .

Summary of parameters and their values:

Model parameters		
$k_{\max\text{poc}}$	0.75	$\text{d}^{-1}$
$k_{\max\text{hmc}}$	0.5	$\text{d}^{-1}$
$Up_{\max}$	2	$\text{d}^{-1}$
$K_{\text{spoc}}$	100	$\text{mmolC.m}^{-3}$
$k_{\text{shmc}}$	5	$\text{mmolC.m}^{-3}$
$K_{\text{sup}}$	0.5	$\text{mmolC.m}^{-3}$
$R_{\text{bas}}$	0.1	$\text{d}^{-1}$
$P_{\text{loss}}$	0.5	-
$rc_{\text{los}}$	0.05	$(\text{mmolC.m}^{-3})^{-1}.\text{d}^{-1}$

Forcing function		
FluxPOC	0.5	mmolC.m <sup>-3</sup> .d <sup>-1</sup>

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 <sup>-3</sup>
HMWC_init	5 mmolC.m <sup>-3</sup>
LMWC_init	0.15 mmolC.m <sup>-3</sup>
BACT_init	5 mmolC.m <sup>-3</sup>

The model is solved numerically using Euler integration:

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

A time step  $\Delta t$  (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  $\Delta t$  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.

# **ANSWERS**

## 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:

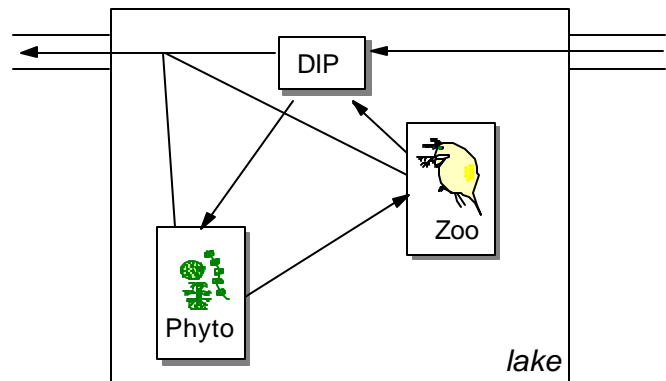
State variables:

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

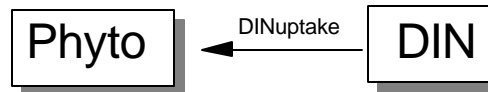
Forcing functions:

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

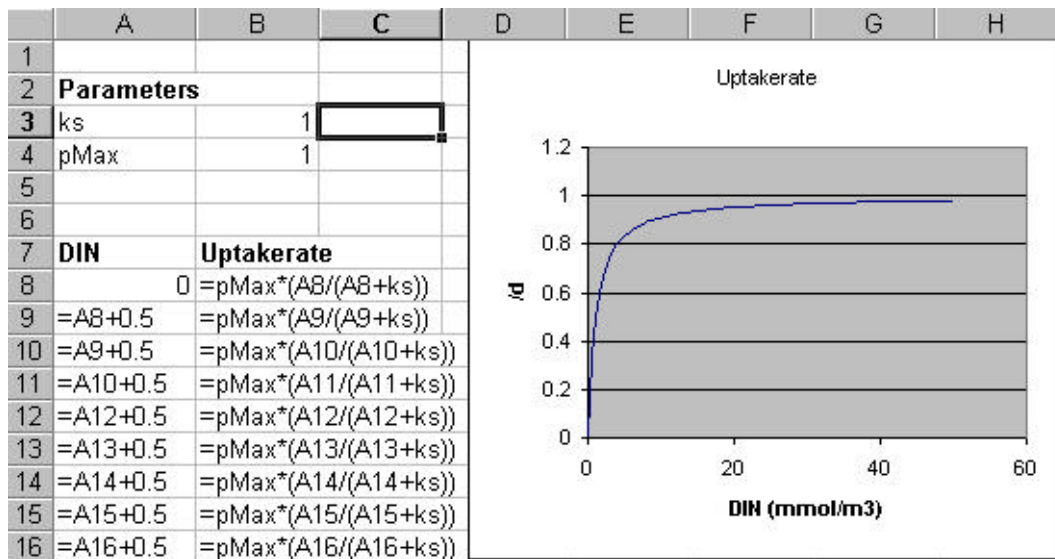
The effect of biomanipulation could be investigated by changing the zooplankton mortality under different flowrate regimes.



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



1. With  $p_{max}$  in  $d^{-1}$ , the units of  $DIN_{uptake\ rate}$  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 ( $\text{mmol N m}^{-3}\text{d}^{-1}$ ) takes into account the concentration of the algae. (the higher algal concentration, the higher the nitrogen uptake rate)

$$\frac{d\text{Phyto}}{dt} = p_{Max} \cdot \frac{\text{DIN}}{\text{DIN} + k_s} \cdot \text{Phyto}$$

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

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

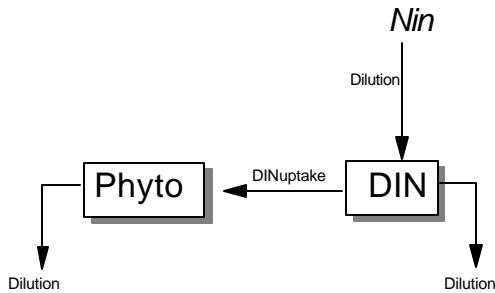
The model is fully specified if we also provide the initial conditions:

$$\text{Phyto}(t_0) = 0.1 \text{ mmol N m}^{-3}$$

$$\text{DIN}(t_0) = 10.0 \text{ mmol N m}^{-3}$$

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:

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

$$\frac{dDIN}{dt} = -p_{max} \cdot \text{Phyto} \cdot \frac{DIN}{DIN + k_s} + \text{Dilrate} \cdot (N_{in} - DIN)$$

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:

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

$$\frac{\mathbf{mmolN} \cdot \mathbf{dm}^{-3}}{\mathbf{d}} = \frac{1}{\mathbf{d}} * \mathbf{mmolN} \cdot \mathbf{dm}^{-3} * \frac{\mathbf{mmolN} \cdot \mathbf{dm}^{-3}}{\mathbf{mmolN} \cdot \mathbf{dm}^{-3} + \mathbf{mmolN} \cdot \mathbf{dm}^{-3}} - \frac{1}{\mathbf{d}} * \mathbf{mmolN} \cdot \mathbf{dm}^{-3}$$

$$\mathbf{mmolN} \cdot \mathbf{dm}^{-3} \cdot \mathbf{d}^{-1} = \mathbf{mmolN} \cdot \mathbf{dm}^{-3} \cdot \mathbf{d}^{-1} - \mathbf{mmolN} \cdot \mathbf{dm}^{-3} \cdot \mathbf{d}^{-1}$$

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.

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

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

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

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.

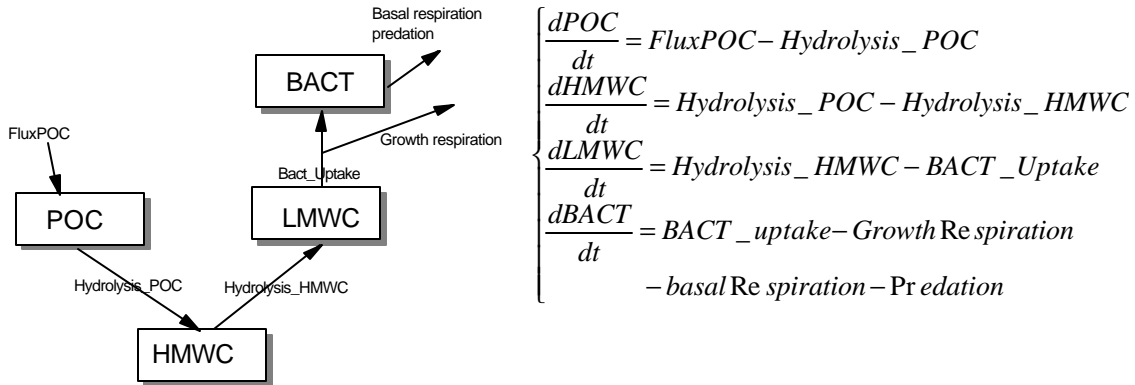
For mass to be conserved in the model, the rate of change of total nitrogen must be equal to inflow-outflow. Mass is indeed conserved by the model equations.

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

	A	B	C	D	E	F	G
1							
2	<b>Parameters</b>						
3		Nin	10				
4		DilRate	0.24				
5		ks	1				
6		pmax	1				
7							
8	N	Gross		Net			
9	0.01	=pmax*A9/(A9+ks)		=B9-DilRate			
10	=Nin/100	=pmax*A10/(A10+ks)		=B10-DilRate			
11	=A10+Nin/100						
12							
13							
14							
15							
16							
17							
18							
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## Exercise 4 Detritus-bacteria model - Solution

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



The mathematical model equations are:

$$\left\{ \begin{array}{l} \frac{dPOC}{dt} = FluxPOC - BACT * k_{max\ poc} * \frac{POC}{POC + k_{spoc}} \\ \frac{dHMWC}{dt} = BACT * k_{max\ poc} * \frac{POC}{POC + k_{spoc}} - BACT * k_{max\ hmw} * \frac{HMWC}{HMWC + k_{shmw}} \\ \frac{dLMWC}{dt} = BACT * k_{max\ hmw} * \frac{HMWC}{HMWC + k_{shmw}} - BACT * UP_{max} * \frac{LMWC}{LMWC + k_{sUp}} \\ \frac{dBACT}{dt} = BACT * UP_{max} * \frac{LMWC}{LMWC + k_{sUp}} * (1 - p_{Loss}) - r_{bas} * BACT - r_{clos} * BACT * BACT \end{array} \right.$$

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 !