OPTIONAL STELLA EXERCISE - NITRIFICATION

This exercise is for the curious and is not a required part of your homework. There will be at least one more optional CEE 3510 exercise during the semester. We will keep track of who turns in optional exercises and this information will be used to provide beneficial consideration for individuals that are on the border line for receiving a higher grade. However, the main benefit is that you get to learn a little more about the environmental field (which we hope is the reason why you are taking this course). Since the grade considerations will be for individuals, please do this on your own and not as part of a team.

It is relatively easy to use STELLA to solve problems like #1 in homework assignment number 4. In fact, since it is a numerical model, STELLA allows us to remove many of the simplifying assumptions inherent in the analytical solution to problem 1. (i.e., no decay of the biological population, and neglect of the nitrite concentration). [Note, if you do this optional assignment you still need to solve problem #1 of assignment #4 using the analytical equations developed in class.]

Here's how to proceed. Since the conversion of ammonia to nitrite and then nitrite to nitrate is a consecutive reaction; you may represent NH$_3$, NO$_2^-$, and NO$_3^-$ as three stocks connected in sequence by flows. Flow out of NH$_3$ should go into NO$_2^-$ and flow out of NO$_2^-$ should go into NO$_3^-$. The rate of each flow is governed by the now familiar kinetic equation:

$$\frac{dS}{dt} = - \frac{kXS}{K_S + S}$$

where S is the concentration of either NH$_3$ or NO$_2^-$ and X is the concentration of Nitrosomonas (M$_{N1}$) or Nitrobacter (M$_{N2}$) bacteria, respectively. [Note: STELLA automatically assigns a negative sign to any flow out of a stock.]

You will need converters for the kinetic coefficients that govern each reaction. Since X can change (i.e. the nitrifying bacterial population may grow and then die away) you also will need stocks for the Nitrosomonas (M$_{N1}$) and Nitrobacter (M$_{N2}$) populations.

The growth of each population (created in STELLA by a flow into the stock) is just the rate of its utilization of substrate times the "yield coefficient" (Y):

$$\frac{dX}{dt} = -Y \frac{dS}{dt} = Y \frac{kXS}{K_S + S}$$

Since you already have stocks for S (either NH$_3$, or NO$_2^-$) and converters for k and K$_S$ (different ones for Nitrosomonas and Nitrobacter), all you need to add are converters for the yield coefficient for each population. Here are some values to try in your model:
For *Nitrosomonas*:  
\[ k_{N1} = 2.25 \text{/day} \]
\[ K_{S1} = 2.1 \text{mg/L} \]
\[ M_{N1}^o = 0.25 \text{mg/L (initial concentration)} \]
\[ Y_{N1} = 0.29 \text{mg Nitrosomonas/mg NH}_3\text{-N} \]

For *Nitrobacter*:  
\[ k_{N2} = 4.0 \text{/day} \]
\[ K_{S2} = 3 \text{mg/L} \]
\[ M_{N2}^o = 0.15 \text{mg/L (initial concentration)} \]
\[ Y_{N2} = 0.084 \text{mg Nitrobacter/mg NO}_2\text{-N} \]

Run your simulation for a time period of 15 days and a time step of 0.001 day. Assume the initial NH\(_3\) concentration is 10 mg/L and the initial concentrations of NO\(_2^-\) and NO\(_3^-\) are zero. If you wish, add converters for velocity and distance so that you can calculate distance downstream as: distance = velocity * time. Use the same velocity as in problem 1 of Problem set #4 (ie., 10 km./day).

Prepare 2 graphs: one with the concentrations of NH\(_3\), NO\(_2^-\), and NO\(_3^-\), and one with the concentrations of *Nitrosomonas* and *Nitrobacter*. Use 10 mg/L as the maximum concentration on the graph for NH\(_3\), NO\(_2^-\), and NO\(_3^-\), and 4 mg/L as the maximum concentration on the graph for *Nitrosomonas* and *Nitrobacter*.

You should see NH\(_3\) decay; a transient concentration of NO\(_2^-\) will appear and disappear, and the ultimate product (NO\(_3^-\)) will accumulate as a function of time (or distance downstream). Compare your answer for NH\(_3\) at a distance of 40 km to the value obtained in problem 1 of problem set #4.

The organism concentration for both *Nitrosomonas* and *Nitrobacter* will increase but never decrease because the above model lets them grow but not die. However, it is easy to include organism death in your model. Create a flow out of your *Nitrosomonas* and *Nitrobacter* stocks. Like the radioactive waste in STELLA exercise #1, we will model cell death as a 1st order process: 
\[
\frac{dX}{dt} = -k_d X
\]

Let the death rate constant (k\(_d\)) for *Nitrosomonas* equal 0.1/day and k\(_d\) for *Nitrobacter* equal 0.05/day. Rerun your simulation. You should now see the bacterial populations slowly decline after attaining maximum values. Notice the effect decay of the bacterial population has on the rate of change of NH\(_3\), NO\(_2^-\), and NO\(_3^-\); do you see why bacterial death can be neglected in the nitrification model?

Those of you who attempt to do this optional problem, please turn in printouts of your STELLA diagrams, equations, tables and graphs for the case where cell death is neglected and the case where it is included. A listing of what to turn in is given on the following page. For your tables use a report interval of one day. We are trying to keep track of who the STELLA enthusiasts are. If there is any help we can give you doing this simulation, don't hesitate to ask!!
### Summary of STELLA output you should turn in.

<table>
<thead>
<tr>
<th>Case</th>
<th>Diagram</th>
<th>Equations</th>
<th>Graphs</th>
<th>Table</th>
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<tr>
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