

Adjusting the Phosphorus Effluent of a Treatment Facility

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Introduction

Ordinary differential equations can often be used in engineering applications to describe the behavior of complex systems as they change with time. One such system can be described by the Michaelis-Menton saturation kinetics equations accounting for the growth rate of algae in the stream (Lang, Lab Handout, 2018). This can be used to create a system of differential equations that models the change in phosphorus and algae concentration with time. A program in FORTRAN was constructed to help a treatment facility reduce their initial phosphorus output of 0.90 (mg/L) into a stream to abide by recreational and drinking water regulations (Lang, Lab Handout, 2018). The regulatory standards state that the phosphorus concentration may not exceed 0.05 (mg/L) at a monitoring point that is 44.5 km downstream. The program will use the Runge-Kutta-Fehlberg method to determine the facilities new maximum initial phosphorus effluent so that regulatory standards are satisfied. Lastly, a sensitivity analysis will be conducted comparing the effects of the average stream velocity, the upstream chlorophyll-A concentration, the removal rate of phosphorus by settling, and the yield coefficient of phosphorus to chlorophyll-A on the initial phosphorus effluent by the treatment facility.

Methodology

The approach used to solve the problem, governing equations used, and description of the algorithm used will be discussed in this section. In order to solve for the final phosphorus concentration 44.5 kilometers downstream, the relationship between the change in phosphorus with time and the change in chlorophyll-A with time must be evaluated. This was done with the Runge-Kutta-Fehlberg

algorithm programmed in a general subroutine with the FORTRAN language. The subroutine evaluated a system of differential equations [1,2] for the current initial phosphorus effluent of 0.9 (mg/L) and initial Chlorophyll-A concentration of 0.002 (mg/L) (Lang, Lab Handout, 2018). This resulted in a relationship between concentration of each compound over the distance downstream. By using this now known value for the final phosphorus concentration, the problem can now be solved in reverse. A search algorithm was used to find the maximum initial phosphorus effluent that the treatment facility can output to still meet the regulatory standards at the point 44.5 kilometers downstream. Below is the system of differential equations that describe the phosphorus [1] and chlorophyll-A [2] concentration in the stream (Lang, Lab Handout, 2018).

$$\frac{dP}{dt} = -K_{P1}P - K_{P2}\mu A \quad [1]$$

$$\frac{dA}{dt} = -K_{A1}A + \mu A \quad [2]$$

Where:

P is the phosphorus concentration (mg/L)

A is the chlorophyll-A concentration (mg/L)

t is the time (days)

K_{P1} is the first-order removal rate of phosphorus by settling (day^{-1})

K_{P2} is the yield coefficient (mg phosphorus/mg chlorophyll-A)

K_{P3} is the half saturation concentration for phosphorus (mg/L)

K_{A1} is the algal death rate (day^{-1})

μ is the algal growth rate (day^{-1}), where $\mu = \mu_{\max} \frac{P}{K_{P3} + P}$

μ_{\max} is the maximum algal growth rate (day^{-1})

The Runge-Kutta-Fehlberg (RKF) algorithm is used to approximate solutions to complex systems that can be described by ordinary differential equations (ODE's) (Ritschel, 3, 2018). The RKF method, unlike the original Runge-Kutta method, uses both a 4th order [3] and a 5th order [4] estimate to find the solution to a differential equation; the results for equation [4] can then be subtracted by [3] to estimate the truncation error (Chapra & Canale, 747, 2015). This was used in the FORTRAN program to increase

the precision of the general solution by controlling the step size. Specifically, the step size is increased if the error is below a threshold of precision and decreased if the error is above this threshold (Chapra & Canale, 748, 2015). This level of control allows the algorithm to converge faster to the solution because it adjusts the step size to an acceptable value when the truncation error is within a user specified range. The values K_1 - K_6 in the RKF algorithm below represent the slope predication at the midpoint of the function that is being evaluated (Chapra & Canale, 740, 2015)

$$y_{i+1} = y_i + \left(\frac{37}{378} K_1 + \frac{250}{621} K_3 + \frac{125}{594} K_4 + \frac{512}{1771} K_6 \right) h \quad [3]$$

$$y_{i+1} = y_i + \left(\frac{2825}{27648} K_1 + \frac{18575}{48384} K_3 + \frac{13525}{55296} K_4 + \frac{277}{14336} K_5 + \frac{1}{4} K_6 \right) h \quad [4]$$

Where,

$$K_1 = f(x_i, y_i)$$

$$K_2 = f\left(x_i + \frac{1}{5}h, y_i + \frac{1}{5}K_1h\right)$$

$$K_3 = f\left(x_i + \frac{3}{10}h, y_i + \frac{3}{40}K_1h + \frac{9}{40}K_2h\right)$$

$$K_4 = f\left(x_i + \frac{3}{5}h, y_i + \frac{3}{10}K_1h - \frac{9}{10}K_2h + \frac{6}{5}K_3h\right)$$

$$K_5 = f\left(x_i + h, y_i - \frac{11}{54}K_1h + \frac{5}{2}K_2h + \frac{70}{27}K_3h + \frac{35}{27}K_4h\right)$$

$$K_6 = f\left(x_i + \frac{7}{8}h, y_i + \frac{1631}{55296}K_1h + \frac{175}{512}K_2h + \frac{575}{13824}K_3h + \frac{44275}{110592}K_4h + \frac{253}{4096}K_5h\right)$$

Application

The RKF algorithm applies to problems that can be modeled with a system of differential equations because it can create higher order estimates from the ODE's describing the relationship. The truncation error associated with the algorithm can also be easily solved for because there are two different order estimates, where the difference in the results will show how much less accurate the lower order estimate is.

The primary problem specific parameters used to describe the relationship are shown below in Table 1. The initial phosphorus and Chlorophyll concentration at the treatment facility, or at a distance 0 (km) downstream, are denoted as $P_{initial}$ and $A_{initial}$, respectively. V is the average velocity of the stream and $Dist.$ is the distance downstream to the monitoring point at which regulatory standards come into effect. K_{P1} is the constant rate at which phosphorus is removed from the stream by settling (Lang, Lab, 2018). K_{P2} is the yield coefficient of phosphorus to chlorophyll-A (Lang, Lab handout, 2018), or essentially the coefficient describing the rate at which the phosphorus is being converted to chlorophyll-A by natural processes. Chlorophyll-A is a way to measure algae concentration in the stream (Lang, Lab handout, 2018). K_{A2} is the rate at which algae dies and is removed from the system. Finally, μ_{max} is a constant describing the maximum rate at which algae will grow in the stream.

Table 1. Parameters used in description of model (Lang, Lab Handout, 2018).

Parameter	$P_{initial}$	$A_{initial}$	V	K_{P1}	K_{P2}	K_{P3}	K_{A1}	μ_{max}	$Dist.$
Value	0.90	0.002	0.06	0.05	1.0	0.03	0.003	0.43	44.5
Units	mg/L	mg/L	m/s	1/day	1/day	1/day	1/day	1/day	Km

Results and Discussion

The FORTRAN program designed to solve this problem produced a new maximum initial phosphorus effluent discharged by the treatment facility of 0.1135 (mg/L) to meet the regulatory limit of 0.05 (mg/L) at the monitoring distance of 44.5 (Km) downstream from the facility. This result indicates that the treatment facility will need to cut its phosphorus effluent significantly at the discharge point, from 0.90 (mg/L) to the determined 0.1135 (mg/L), to meet recreational and drinking water standards. The program also produced the values necessary to create a plot of the relationship between the new

and old phosphorus and chlorophyll-A concentrations over the distance downstream from the discharge point to the monitoring point. This relationship can be seen in Figure 1.

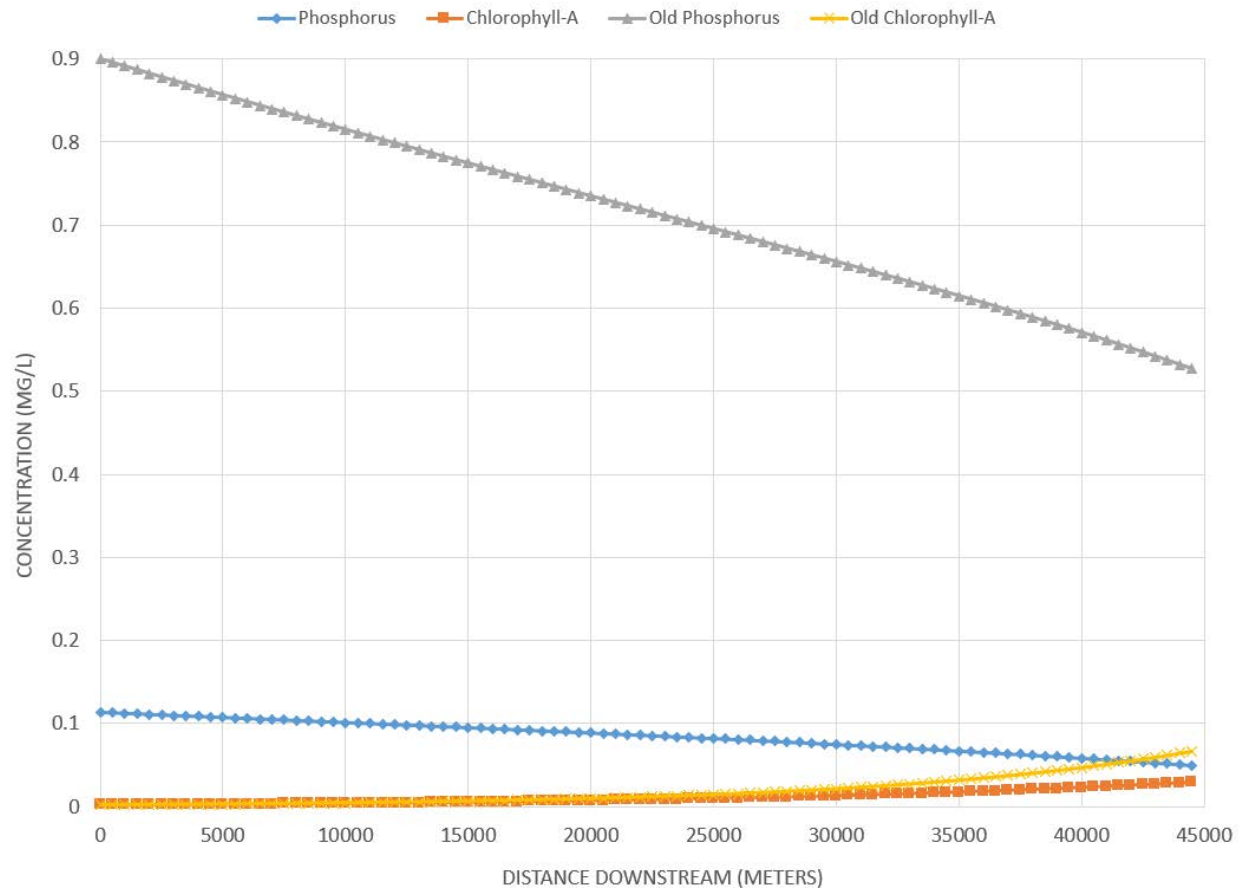


Figure 1: Relationship between phosphorus and chlorophyll-A concentrations plotted over the distance from the discharge point to the monitoring point.

The plot above shows that the old phosphorus begins at a much higher initial value, but it decreases at a much faster rate than the new phosphorus levels. The Chlorophyll-A increases at an exponential rate, presumably to come to an unknown equilibrium level with the changing phosphorus concentration. The old Chlorophyll-A concentration is found to be increasing much faster as its growth is dependent on the old, much higher, phosphorus levels present in the stream (Lang, Lab handout, 2018). This shows that by decreasing the initial phosphorus levels at the discharge point one can drastically reduce the rate at which algae will grow. This is important because algal blooms can introduce toxins

(blue-green algae) in the water and this can negatively affect aquatic life and the safety of others using the watershed (Cashman, Lecture, 2016). In addition, excess algae can decrease the dissolved oxygen in the stream, which is an important attribute when assessing water quality (Otero, Lab Lecture, 2018). Finally, a sensitivity analysis (Figure 2) was performed on the initial Chlorophyll-A, average velocity, the removal rate of phosphorus by settling (K_{P1}), and the yield coefficient of phosphorus to chlorophyll-A (K_{P2}).

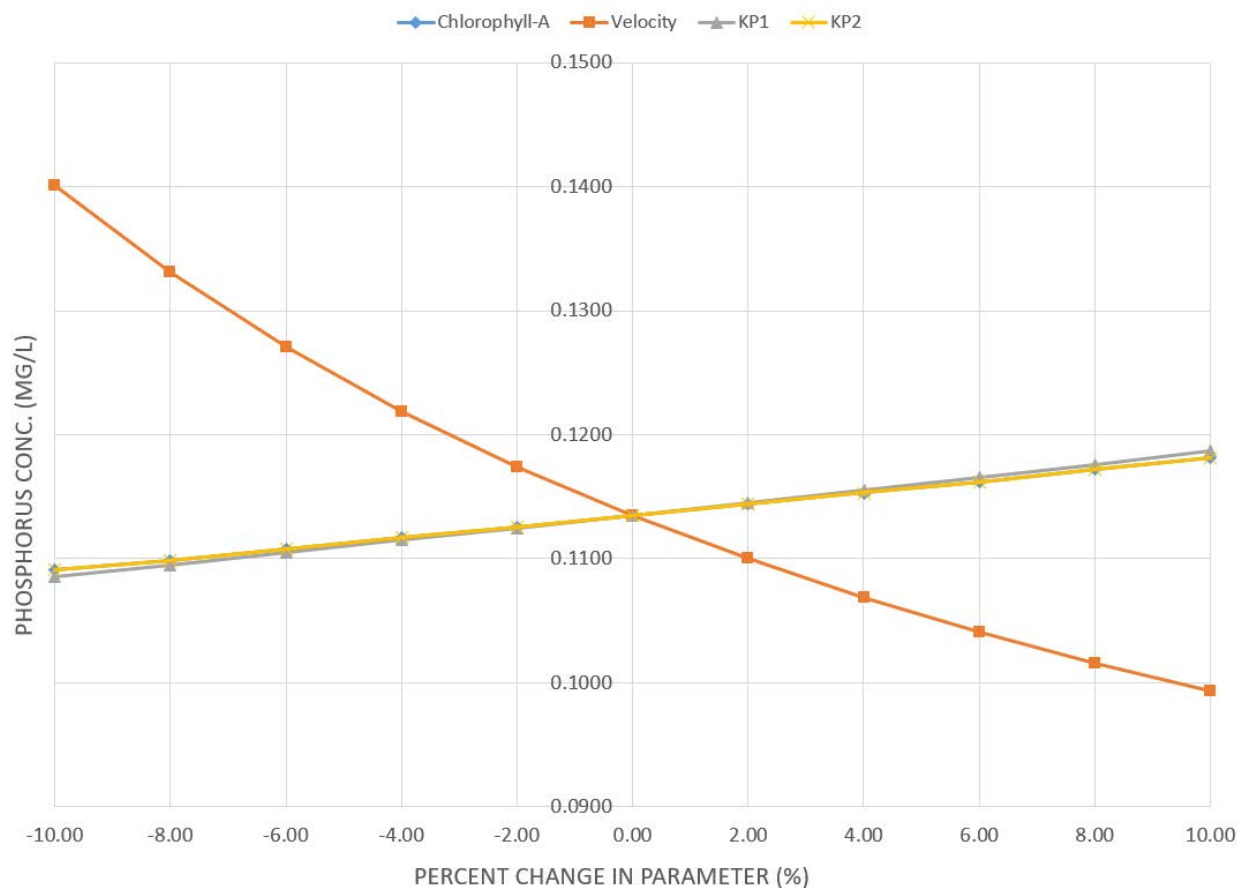


Figure 2: Sensitivity analysis shows how the chlorophyll-A, average velocity, removal rate of phosphorus by settling (K_{P1}), and the yield coefficient of phosphorus to chlorophyll-A (K_{P2}) affect the initial allowable phosphorus effluent.

The sensitivity analysis indicates that the most efficient way to increase the initial allowable phosphorus concentration is by decreasing the velocity in the river. Vice versa, is also true, in that increasing the velocity would also greatly decrease the initial allowable phosphorus concentration. Two parameters analyzed, the chlorophyll-A and the yield coefficient, had the same affect on the phosphorus effluent. This makes sense because yield coefficient is the rate at which phosphorus is converted to chlorophyll-A and a higher initial chlorophyll-A concentration would allow more phosphorus to be converted resulting in the same affect on the phosphorus concentration. Lastly, the removal rate of phosphorus by settling also happens to produce a very similar effect on the initial concentration.

Conclusions

Differential equations are often used in engineering applications to model the relationships of complex phenomenon. The Runge-Kutta-Fehlberg method was used in a FORTRAN program to estimate the solution to a system of differential equations. The program determined that, to meet the standard of 0.05 (mg/L) at the monitoring point, the treatment facility must reduce their phosphorus discharge to a maximum of 0.1135 (mg/L). In addition, the relationship between phosphorus and chlorophyll-A concentration was more thoroughly understood through a plot over the distance downstream. The sensitivity analysis showed that the average velocity on the stream has the largest impact on the allowable phosphorus discharge to meet regulations. Should the topic need be explored further, one could use the FORTRAN program to determine the distance necessary for the phosphorus and chlorophyll-A concentrations to reach an equilibrium with one another.

References

Ritschel, T. (2013). *Numerical Methods For Solution of Differential Equations*. Technical University of Denmark, Kongens Lyngby, Denmark. (pg. 3)

Chapra, S. C., and Canale, R. P. (2015). *Numerical methods for engineers*. McGraw-Hill Education, New York, NY. (ch. 25, pgs. 740, 747, 748.)

Appendix

Table 2. Sensitivity analysis of velocity on phosphorus concentration

Velocity		
% Change	Δ	P
-10.00	0.0540	0.1401
-8.00	0.0552	0.1331
-6.00	0.0564	0.1271
-4.00	0.0576	0.1219
-2.00	0.0588	0.1174
0.00	0.0600	0.1135
2.00	0.0612	0.1100
4.00	0.0624	0.1069
6.00	0.0636	0.1041
8.00	0.0648	0.1016
10.00	0.0660	0.0993

Table 3. Sensitivity analysis of chlorophyll-A on phosphorus concentration

Chlorophyll-A		
% Change	Δ	P
-10.00	0.001800	0.1091
-8.00	0.001840	0.1099
-6.00	0.001880	0.1108
-4.00	0.001920	0.1117
-2.00	0.001960	0.1126
0.00	0.002000	0.1135
2.00	0.002040	0.1144
4.00	0.002080	0.1153
6.00	0.002120	0.1162
8.00	0.002160	0.1172
10.00	0.002200	0.1181

Table 4. Sensitivity analysis of settling removal rate on phosphorus concentration

K_{P1}		
<i>% Change</i>	Δ	<i>P</i>
-10.00	0.0450	0.1086
-8.00	0.0460	0.1095
-6.00	0.0470	0.1105
-4.00	0.0480	0.1115
-2.00	0.0490	0.1125
0.00	0.0500	0.1135
2.00	0.0510	0.1145
4.00	0.0520	0.1155
6.00	0.0530	0.1166
8.00	0.0540	0.1176
10.00	0.0550	0.1187

Table 5. Sensitivity analysis of the yield coefficient on phosphorus concentration

K_{P2}		
<i>% Change</i>	Δ	<i>P</i>
-10.00	0.90	0.1091
-8.00	0.92	0.1099
-6.00	0.94	0.1108
-4.00	0.96	0.1117
-2.00	0.98	0.1126
0.00	1.00	0.1135
2.00	1.02	0.1144
4.00	1.04	0.1153
6.00	1.06	0.1162
8.00	1.08	0.1172
10.00	1.10	0.1181

Program Execution and Output

Script started on 2018-10-15 15:58:44-0700;

jdt385@CNRS-LinuxMint: ~/Documents[01;

jdt385@CNRS-LinuxMint[00m:[01;34m~/Documents; gfortran final.f90 -o f.exe

jdt385@CNRS-LinuxMint: ~/Documents;

jdt385@CNRS-LinuxMint[00m:[01;34m~/Documents; ./f.exe

Initial phosphorus concentration is 0.9 (mg/L) for the table below

Distance	Phosphorus	Chlorophyl
500.00000000000006	0.89558845710665480	2.0812956190132213E-003
1000.00000000000001	0.89119485482432736	2.1658817755978370E-003
1500.00000000000000	0.88681894991077459	2.2538911171083756E-003
2000.00000000000002	0.88246051868586239	2.3454615048452824E-003
.		
.		
.		
43000.0000000000073	0.54203554676463761	5.9753551650615098E-002
43500.0000000000073	0.53703953505140700	6.2129968107531401E-002
44000.0000000000080	0.53197382937781534	6.4599637685314751E-002
44500.0000000000073	0.52683517995430607	6.7166126570171070E-002

Current phosphorus concentration at 44.5 (km) is 0.52683517995430607 (mg/L)

Current initial concentration of 0.89999997615814209 (mg/L)

Begin search algorithm for new initial Phosphorus concentration

0.87999997660517693

0.85999997705221176

0.83999997749924660

0.81999997794628143

0.79999997839331627

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0.11269999371870654

0.11279999371618032

0.11289999371365411

0.11299999371112790

0.11309999370860169

0.11319999370607547

0.11329999370354926

0.11339999370102305

0.11349999369849684

Success! results below

The new initial phosphorus concentration is shown in the table below

Distance	Phosphorus	Chlorophyl

500.00000000000006	0.11288746732706378	2.0660583355757677E-003
1000.00000000000001	0.11227577120456855	2.1342188088834782E-003
1500.00000000000000	0.11166483728888392	2.2045450991896895E-003
2000.00000000000002	0.11105459607648083	2.2771025651589149E-003
.		
.		
.		
43000.0000000000073	5.2925415099906468E-002	2.6797227801933228E-002
43500.0000000000073	5.1956257881906748E-002	2.7505627780904113E-002
44000.0000000000080	5.0977955270582347E-002	2.8227662088285595E-002
44500.0000000000073	4.9990630109432416E-002	2.8963247766327201E-002

Final Report:

Final phosphorus concentration at 44.5 (km) is 4.9990630109432416E-002 (mg/L)

New initial phosphorus concentration: 0.11349999369849684 (mg/L)

Parameters:

velocity= 5.999999999999998E-002 (m/s)

distance= 44500.000000000000 (meters)

tend= 8.5841049382716204 (days)

nsteps= 89

timereport= 9.6450617283950629E-002 (days)

reportinteger= 500.00000000000000 (meters)

Program has finished running.