Hydrodynamic-Sediment-Phosphorus interaction: A mathematical control approach

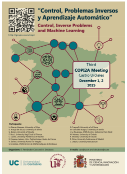
(Funded by Project TED2021-129324B-I00)

Lino J. Alvarez-Vázquez*,

Aurea Martínez*, Miguel E. Vázquez-Méndez**

*** Departamento de Matemática Aplicada II**
Universidade de Vigo

** Departamento de Matemática Aplicada
Universidade de Santiago de Compostela



Group of Simulation & Control

https://gscpage.wordpress.com

Table of contents

Introduction

Motivation

Mathematical modelling is an effective tool for studying water quality in rivers or channels, and management and operation of reservoirs created by dams in these.

Motivation

These models should include phosphorus transport (one of the key nutrients affecting eutrophication) and sediment particles (since most phosphorus in water are adsorbed by sediment particles and transported in the particulate phase).

Internal phosphorus loading in rivers and channels refers to phosphorus contained in bottom sediments and which, under certain conditions such as hypoxia or pH/temperature changes, can be released into the water column, continuing or exacerbating pollution and eutrophication problems even after controlling external sources of phosphorus.

Motivation

Release of phosphorus from sediment is a slow process that occurs in the interstitial water and can cause uncontrolled algal growth and a decrease in dissolved oxygen.

This release of previously settled phosphorus from sediments into the water column of rivers and channels often occurs when anoxic conditions arise. This process can significantly hinder lake restoration efforts by providing a long-term source of phosphorus that continues to fuel algal blooms long after external nutrient loads are reduced.

Objectives

In this talk we deal with a model that incorporates sediment-phosphorus interactions to the 1D hydrodynamic model.

Our main aim is related to controlling different parameters in the model in order to maximize several possible objectives (hydropower generation in associated dams, flood reduction, etc.), while minimizing nutrient concerns (related to pollution levels and eutrophication) and/or sedimentation (cause of capacity reduction and malfunction).

Mathematical modeling

State variables

- $A(x,t)$: wet area, for $(x,t) \in (0,L) \times (0,T)$
- $u(x,t)$: averaged velocity of water
- $Q(x,t)$: water flux ($Q = Au$)
- $A_s(x,t)$: settled area
- $z(x,t)$: heigth of sediment ($z = \tilde{B}(A_s)$)
- $H(x,t)$: heigth of water ($H = \tilde{B}(A + A_s) - \tilde{B}(A_s)$)
- $S(x,t)$: averaged concentration of suspended particles of non-cohesive sediment
- $C_w(x,t)$: averaged concentration of phosphorus (P) dissolved in water
- $C_s(x,t)$: averaged concentration of P in suspended particles
- $C_b^1(x,t)$: averaged concentration of P in the aerobic layer of sediment
- $C_b^2(x,t)$: averaged concentration of P in the anaerobic layer

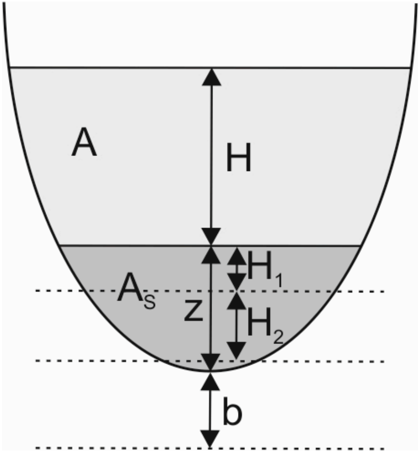


Figure: Channel section

Hydrodynamic model

$$\begin{cases} \dfrac{\partial A}{\partial t} + \dfrac{\partial Q}{\partial x} = 0 \quad \text{in } (0,L)\times(0,T) \\ \dfrac{\partial Q}{\partial t} + \dfrac{\partial}{\partial x}\left(\dfrac{Q^2}{A}\right) + gA\dfrac{\partial}{\partial x}(b+z+H) + \dfrac{gP}{C^2}\dfrac{Q|Q|}{A^2} = 0 \end{cases} \tag{1}$$

where:

- L: length of channel
- g: gravity acceleration
- $b(x)$: geometry of the river bottom (bathymetry)
- P: wetted perimeter
- C: Chézy friction coefficient

Non-cohesive sediment model

$$\begin{cases} \dfrac{\partial(AS)}{\partial t} + \dfrac{\partial(QS)}{\partial x} - \dfrac{\partial}{\partial x}\left(k_1 A \dfrac{\partial S}{\partial x}\right) - \dfrac{Q}{L_A}(S^* - S) = 0 \\ \rho_s(1-\varepsilon)\dfrac{\partial A_s}{\partial t} = -\dfrac{Q}{L_A}(S^* - S) \end{cases} \tag{2}$$

where:

- k_1: diffusion coeficient
- L_A: adaptation length (depending on settling velocity and hydraulic radius)
- S^*: sediment transport capacity
- ρ_s: density of sediment particles
- ε: porosity of the bottom sediment

Phosphorus model

$$
\begin{cases}
\dfrac{\partial(AC_w)}{\partial t} + \dfrac{\partial(QC_w)}{\partial x} - \dfrac{\partial}{\partial x}\left(k_1 A \dfrac{\partial C_w}{\partial x}\right) + \lambda A C_w = S_w \\
\dfrac{\partial(ASC_s)}{\partial t} + \dfrac{\partial(QSC_s)}{\partial x} - \dfrac{\partial}{\partial x}\left(k_1 A \dfrac{\partial(SC_s)}{\partial x}\right) = S_s \\
BH_1 \dfrac{\partial C_b^1}{\partial t} = S_b^1 \\
BH_2 \dfrac{\partial C_b^2}{\partial t} = S_b^2
\end{cases}
\tag{3}
$$

where:

- λ: net algal uptake rate of phosphorus (related to eutrophication)
- B: channel width
- H_1, H_2: thickness of aerobic and anaerobic active sediment layers
- S_w, S_s, S_b^1, S_b^2: various sources of phosphorus

These source terms can be written as:

$$
\begin{aligned}
S_w &= R_1 - R_2 - R_3 - R_6 + R_8 \\
S_s &= R_2 - R_7 + R_9 \\
S_b^1 &= R_3 - (R_4 + R_5) + (R_6 + R_7) - (R_8 + R_9) - (R_{10} - R_{11}) \\
S_b^2 &= (R_4 + R_5) + (R_{10} - R_{11}) - (R_{12} - R_{13})
\end{aligned}
$$

Term R_1 stands for external phosphorus emissions (also including anthropogenic sources: industrial, domestic, agricultural...)

Terms R_2 - R_5 depend on the relations between the different concentrations of phosphorus in the corresponding layers.

Terms R_6 - R_{13} depend on the type of riverbed deformation, that is, whether there is sediment deposition ($\frac{\partial A_s}{\partial t} > 0$), or sediment erosion ($\frac{\partial A_s}{\partial t} < 0$).

To illustrate the different type of sources, we show for example the expressions for:

R_2: Adsorption of phosphorus by suspended sediment

$$R_2 = ASk_2(K_{ads}C_w - C_s)$$

R_7: Sediment deposition from phosphorus in suspended particles

$$R_7 = \begin{cases} \rho_s(1-\varepsilon)\frac{\partial A_s}{\partial t}C_s & \text{if } \frac{\partial A_s}{\partial t} \geq 0 \\ 0 & \text{if } \frac{\partial A_s}{\partial t} < 0 \end{cases}$$

Initial conditions

$$
\begin{cases}
A(x,0) = A^0(x) & \text{in } (0,L) \\
Q(x,0) = Q^0(x) & \\[6pt]
S(x,0) = S^0(x) & \\
A_s(x,0) = A_s^0(x) & \\[6pt]
C_w(x,0) = C_w^0(x) & \\
C_s(x,0) = C_s^0(x) & \\
C_b^1(x,0) = C_b^{1,0}(x) & \\
C_b^2(x,0) = C_b^{2,0}(x) &
\end{cases}
\tag{4}
$$

Boundary conditions

$$\left\{\begin{array}{l} A(L,t) = A_L(t) \quad \text{in } (0,T) \\ Q(0,t) = Q_0(t) \\ \\ S(0,t) = S_0(t) \\ \dfrac{\partial S}{\partial x}(L,t) = S_L(t) \\ \\ C_w(0,t) = C_{w,0}(t) \\ \dfrac{\partial C_w}{\partial x}(L,t) = C_{w,L}(t) \\ C_s(0,t) = C_{s,0}(t) \\ \dfrac{\partial (SC_s)}{\partial x}(L,t) = C_{s,L}(t) \end{array}\right. \tag{5}$$

For the particular case of a channel with rectangular section of width B, a non-conservative formulation could read:

$$\begin{cases} \dfrac{\partial A}{\partial t} + \dfrac{\partial Q}{\partial x} = 0 \\ \dfrac{\partial Q}{\partial t} + \dfrac{\partial}{\partial x}\left(\dfrac{Q^2}{A}\right) + \dfrac{g}{B}\dfrac{\partial}{\partial x}\left(\dfrac{A^2}{2}\right) + g\left(\dfrac{\partial b}{\partial x} + \dfrac{1}{B}\dfrac{\partial A_s}{\partial x}\right) A + \dfrac{gP}{C^2}\dfrac{Q|Q|}{A^2} = 0 \end{cases}$$

$$\begin{cases} \dfrac{\partial S}{\partial t} + \dfrac{\partial}{\partial x}\left(\dfrac{QS}{A}\right) - \dfrac{\partial}{\partial x}\left(k_1 \dfrac{\partial S}{\partial x}\right) - \dfrac{1}{A}\dfrac{Q}{L_A}(S^* - S) = 0 \\ \dfrac{\partial A_s}{\partial t} = -\dfrac{1}{\rho_s(1-\varepsilon)}\dfrac{Q}{L_A}(S^* - S) \end{cases}$$

$$\begin{cases} \dfrac{\partial C_w}{\partial t} + \dfrac{\partial}{\partial x}\left(\dfrac{QC_w}{A}\right) - \dfrac{\partial}{\partial x}\left(k_1 \dfrac{\partial C_w}{\partial x}\right) + \lambda C_w = \dfrac{S_w}{A} \\ \dfrac{\partial (SC_s)}{\partial t} + \dfrac{\partial}{\partial x}\left(\dfrac{QSC_s}{A}\right) - \dfrac{\partial}{\partial x}\left(k_1 \dfrac{\partial (SC_s)}{\partial x}\right) = \dfrac{S_s}{A} \\ \dfrac{\partial C_b^1}{\partial t} = \dfrac{S_b^1}{BH_1} \\ \dfrac{\partial C_b^2}{\partial t} = \dfrac{S_b^2}{BH_2} \end{cases}$$

$+$ Initial Conditions (4)

$+$ Boundary Conditions (5)

In several cases, diffusion effects can be considered negligible (that is, $k_1 = 0$).

Then, above system can be rewritten in the standard notation of a balance law:

$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x} K(U) = C(U, x)$$

where:

$$U = \begin{pmatrix} A \\ Q \\ S \\ A_s \\ C_w \\ SC_s \\ C_b^1 \\ C_b^2 \end{pmatrix}, \qquad K(U) = \begin{pmatrix} Q \\ \frac{Q^2}{A} + \frac{g}{2B}A^2 \\ \frac{QS}{A} \\ 0 \\ \frac{QC_w}{A} \\ \frac{QSC_s}{A} \\ 0 \\ 0 \end{pmatrix}$$

$$C(U,x) = \begin{pmatrix} 0 \\ -g\frac{\partial b}{\partial x} - \frac{A}{B}\frac{\partial A_s}{\partial x} - \frac{gP}{C^2}\frac{Q|Q|}{A^2} \\ \frac{1}{L_A}\frac{Q}{A}(S^* - S) \\ \frac{1}{\rho_s(1-\varepsilon)L_A}Q(S^* - S) \\ \frac{S_w}{A} - \lambda C_w \\ \frac{S_s}{A} \\ \frac{S_b^1}{BH_1} \\ \frac{S_b^2}{BH_2} \end{pmatrix}$$

In order to study the hyperbolicity of the non-diffusion system we have that its full eigenstructure corresponds to the eigenvalues of the Jacobian matrix of K:

$$\begin{cases} \lambda_1 = \dfrac{Q}{A} + \sqrt{\dfrac{g}{B}A} = u + \sqrt{gH} \\ \lambda_2 = \dfrac{Q}{A} - \sqrt{\dfrac{g}{B}A} = u - \sqrt{gH} \\ \lambda_3 = \lambda_5 = \lambda_6 = \dfrac{Q}{A} = u \\ \lambda_4 = \lambda_7 = \lambda_8 = 0 \end{cases}$$

However, to pose a realistic problem, in the remainder of this work we will include diffusion effects.

Work in progress

Let us consider the case where at the end of the channel there exists a dam that allows the reservoir water level to be regulated, for example, by means of an outlet intended for energy production in a hydroelectric power plant.

Obviously, the greater the water discharge, the greater the electricity production. Nevertheless, excessive water discharge could harm the water quality in the system or make difficult the future refill possibility.

An optimal control problem

In this work we are interested in finding the optimal water level at the end of the channel (corresponding to the reservoir water level) so that the energy production is maximized (this would be equivalent to minimizing the wet area at the end of the channel), but at the same time the final concentration of dissolved phosphorus in the water is minimized (in order to reduce the possible harmful effects of eutrophication).

On the other hand, it is important that the wet zone at final end remains within certain minimum and maximum thresholds for the system to function properly (storage capacity, water quality. . .).

Mathematical formulation

* Design variable: A_L (in a first phase assumed constant)

* Cost function: $J(A_L) = \alpha\, A_L + \int_0^L C_w(T)\, dx$

(weight parameter $\alpha > 0$)

* Control constraints: $A_{min} \leq A_L \leq A_{max}$

Optimal control problem

$$\min_{A_{min} \leq A_L \leq A_{max}} J(A_L)$$

Current and future work:

- Theoretical analysis of the problem: existence of optimal solutions, optimality conditions. . .
- Computational resolution of the state systems
- Numerical optimization of the problem
- Inclusion of state constraints
- Control depending on time $A_L(t)$ (for instance, piecewise constant)
- Other design variables and/or cost functions
- . . .

Preliminary numerical experiences

Numerical simulation

The first step consists in the numerical solving of the hydrodynamic/ sedimentation systems. To compute the discretized A, Q, S, A_s we use here our own Fortran software correponding to a Lagrange P_1 finite element technique combined with an implicit time discretization, incorporating the method of characteristics for the convective terms.

Then, we solve the phosphorus model in a similar manner to obtain the discretized C_w, C_s, C_b^1, C_b^2.

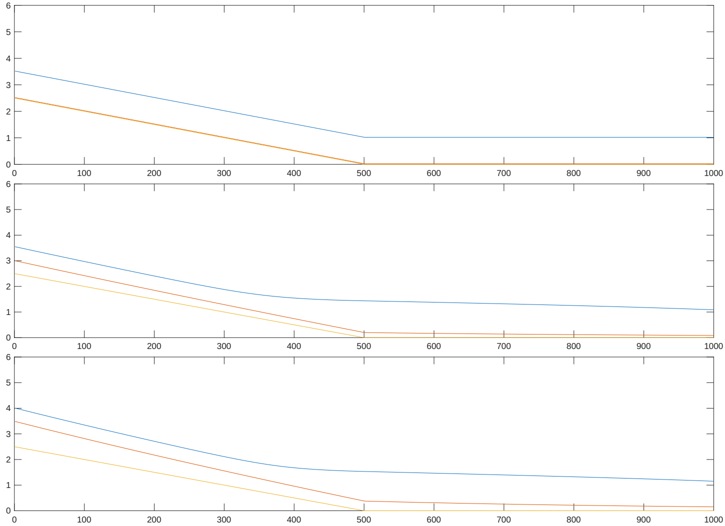
Numerical optimization

Once computed the discrete state variables, we can compute the discretized cost function $J(A_L)$ by means of any cuadrature rule.

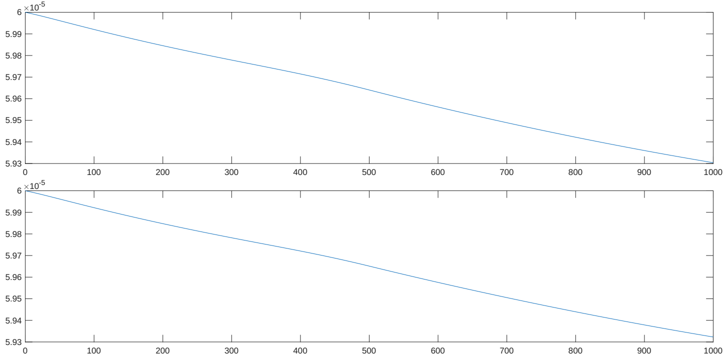
Finally, the solution of the discrete, bound-constrained minimization problem can be obtained by any numerical minimization algorithm (eventually after inclusion of a penalty term to deal with the bound constraints of the design variables):

- Derivative-free algorithms: direct search, genetic, random search. . .
- Gradient-type algorithms, with gradient approximated by finite differences (since adjoint techniques seem too complex here).

$$b(x) + z(x,t) + H(x,t), \qquad t = 0,\ \frac{T}{2},\ T.$$



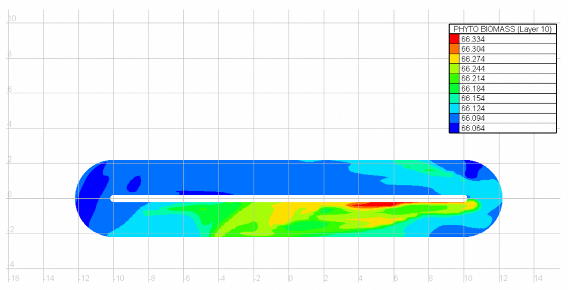
$$C_w(x,t), \qquad t = \frac{T}{2},\ T.$$



Further details

- L.J. Alvarez-Vázquez, G. Casal, A. Martínez, M.E. Vázquez-Méndez. "A novel formulation for designing a monitoring strategy: Application to the design of a river quality monitoring system", *Environ. Model. Assess.*, 22, pp. 279 - 289, 2017.
- L.J. Alvarez-Vázquez, A. Martínez, C. Rodríguez, M.E. Vázquez-Méndez. "Sediment minimization in canals: An optimal control approach", *Math. Comput. Simul.*, 149, pp. 109 - 122, 2018.
- L.J. Alvarez-Vázquez, A. Martínez, C. Rodríguez, M.E. Vázquez-Méndez, M.A. Vilar. "Mathematical analysis and optimal control of heavy metals phytoremediation techniques", *Appl. Math. Model.*, 73, pp. 387 - 400, 2019.
- F.J. Fernández, A. Martínez, L.J. Alvarez-Vázquez. "Controlling eutrophication by means of water recirculation: An optimal control perspective", *J. Comput. Appl. Math.*, 421, 114886, 2023.
- L.J. Alvarez-Vázquez, A. Martínez, M.E. Vázquez-Méndez. Work in progress.

Recent topics: 1 - Optimal management of raceway ponds for bioenergy production

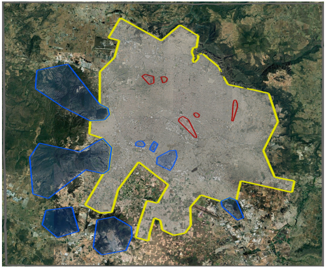


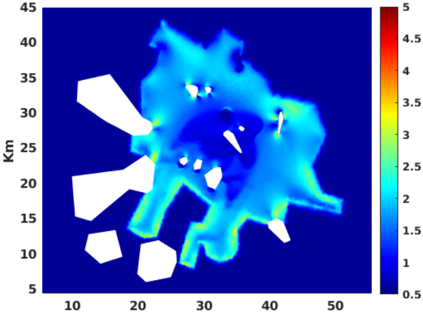
Other recent topics

Optimal management of raceway ponds for bioenergy production

- A. Martínez, L.J. Alvarez-Vázquez, C. Rodríguez, M.E. Vázquez-Méndez. "Algal cultivation for bioenergy production: First mathematical modeling results in raceways", *XI International Conference on Adaptive Modeling and Simulation (ADMOS 2023)*, Gothenburg, 2023.
- — "Preliminary numerical results in the optimization of bioenergy-intended raceway ponds", in *Numerical Mathematics and Advanced Applications ENUMATH 2023, Vol. 2* (A. Sequeira et al., eds.), pp. 153 - 161, Springer, 2025.
- — "Optimizing algaculture in open-channel raceway ponds for the production of bioenergy", submitted, 2025.

2 - Control of air pollution in an urban-porous city



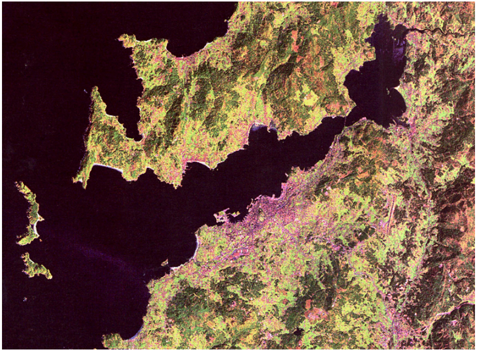


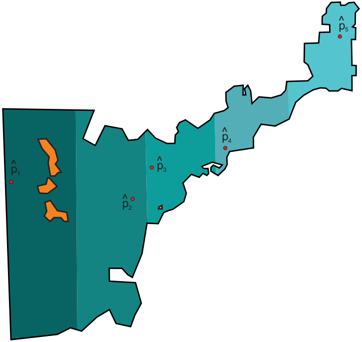
Other recent topics

Control of air pollution in an urban-porous city

- N. García-Chan, L.J. Alvarez-Vázquez, A. Martínez, M.E. Vázquez-Méndez. "A nonconservative macroscopic traffic flow model in a two-dimensional urban-porous city", *Math. Comput. Simul.*, 233, pp. 60 - 74, 2025.
- — "A multi-model study of the air pollution related to traffic flow model in a two-dimensional porous metropolitan area", *J. Comput. Appl. Math.*, 473, 116903, 2026.
- — Work in progress.

3 - Water pollution monitorization



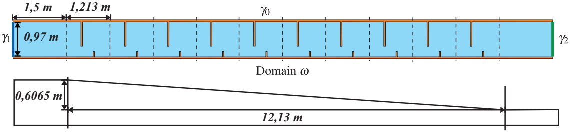


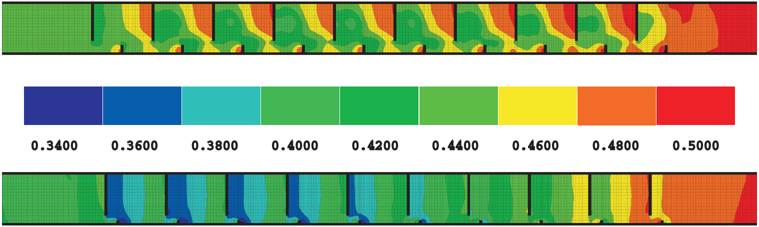
Other recent topics

Water pollution monitorization

- L.J. Alvarez Vázquez, A. Martínez, C. Rodríguez, M.E. Vázquez Méndez. "Optimal design of an estuarine water health monitoring network by means of optimal control techniques", in *Numerical Mathematics and Advanced Applications ENUMATH 2023, Vol. 1* (A. Sequeira et al., eds.), pp. 65 - 72, Springer, 2025.

4 - Sustainable Development Goals (2030 Agenda)





Other recent topics

Sustainable Development Goals (2030 Agenda)

- M.E. Vázquez Méndez, L.J. Alvarez Vázquez, N. García Chan, A. Martínez, C. Rodríguez. "Mathematics for Optimal Design of Sustainable Infrastructure", *18th International Conference on Environmental Science and Technology (CEST 2023)*, Athens, 2023.
- — "Mathematics for Optimal Design of Sustainable Infrastructures", *Euro-Mediterranean J. Environ. Integration*, 9, pp. 989 - 996, 2024.

Hydrodynamic-Sediment-Phosphorus interaction: A mathematical control approach
(Funded by Project TED2021-129324B-I00)

Lino J. Alvarez-Vázquez*,

Aurea Martínez*, Miguel E. Vázquez-Méndez**

*** Departamento de Matemática Aplicada II**
Universidade de Vigo

** Departamento de Matemática Aplicada
Universidade de Santiago de Compostela

GSC Group of Simulation & Control

https://gscpage.wordpress.com