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NUMERICAL MODELING OF BIOCHEMICAL TRANSPORT PROCESSES WITH HETEROGENEOUS SOURCE TERMS. APPLICATION TO WASTEWATER MODELS.

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Abstract. *Subsurface flow constructed wetlands are one of the different types of wastewater treatments used nowadays. There, water is treated by physical, biological and chemical processes while flowing through a porous media. Many aspects of detailed processes which take place there are not well-known. In fact, a key point of their behavior is that simultaneously aerobic and anaerobic conditions take place in different parts of the domain. Mathematically the problem is a Convection – Diffusion – Reaction system of equations, highly coupled because of the nonlinear reaction term that models the biochemical processes. An stabilized Galerkin formulation is used for spatial discretization, and the Runge-Kutta-Fehlberg 4-5 scheme is used for time integration. Homogeneous examples with and without oxygen entrance throughout all domain have been used to check the numerical performance of the approach. The Activated Sludge Model No.1 (ASM1) and a six–equations model based on it are used as examples of complex reaction models. Two dimensional examples with oxygen entrance in just part of the domain have been also computed. It has been check that under horizontal low–velocity conditions a discontinuity in oxygen vertical profile is found, even if continuous transition in oxygen entrance is imposed. In this situation, classical convection stabilization has shown to be usefulness to smooth discontinuities produced by source terms. Further numerical improvements needed are indicated, as well as an extension to more realistic biochemical models for subsurface flow constructed wetlands.*

1 INTRODUCTION

There are different wastewater treatments, but all of them have the aim of returning water after its use to the environment without the pollutants which can damage it and our health. Those are traditionally classified as primary, secondary and tertiary treatment. The first one refers to the physical processes to separate the solids suspended in water. The secondary treatment, which can be made by biological or chemical processes, removes most of the organic matter. And the last treatment is used to remove other constituents that are not significantly reduced on the previous ones.

The numerical modeling of the subsurface flow constructed wetlands is the motivation of this work. They are part of the named "natural systems" for wastewater treatment. They consist on lagoons or channels, which are planted with humid zone plants. In those wetlands water is treated simultaneously by physical, chemical and biological processes [7]. Due to the combination of these processes, that are common on the "natural systems", water quality is similar to or even better than that coming out from a tertiary treatment [2].

Different aspects of the processes given on those wetlands are still a *black box* [7]. Although a biological model of wastewater processes is already developed, and some mathematical modeling of it has been achieved, those models are not valid as stated now for its use on subsurface flow wetlands. One of the problems when trying to understand the wetlands operation is knowing whether aerobic or anaerobic conditions are given. Oxygen not only enters the wetlands solved in water and through the free surface, but also through the plants existing on those wetlands. Thus, on the superior part of wetlands, aerobic processes take place, while on the inferior part, anaerobic processes are the ones in action.

This work focus in the numerical modeling of this situation, a biochemical model with an heterogeneous source term. The outline follows. First, a brief review of the mathematical model is presented. Next, the key points of the numerical solver are explained. As the unsteady problem is considered, both spatial and time discretization are needed. In contrast with usual approached by finite differences, see [9] and [5], here a stabilized finite element approach is proposed. Numerical formulation is briefly detailed, material parameters used in examples presented, and first results with a simplified six-variables model analyzed. After that a brief discussion about convection stabilization is summarized. And then, results obtained with the ASM1 model applied to homogeneous and heterogeneous two dimensional problems are presented and analyzed. Contribution finishes with main conclusions of the overall analysis. Capabilities and limits of the proposed approach are highlighted.

2 MATHEMATICAL MODEL

The system of equations which govern Convection – Diffusion – Reaction processes can be expressed as

$$\frac{\partial \mathbf{c}}{\partial t} = \nabla \cdot (\nu \nabla \mathbf{c}) - \mathbf{u} \cdot \nabla \mathbf{c} + \boldsymbol{r}(\boldsymbol{c}) \qquad \text{in } \Omega \text{ x }]0, T[\tag{1}$$

with t representing time, $\mathbf{c}$ the vector of unknowns, $\mathbf{u}$ the velocity field, $\boldsymbol{r}(\boldsymbol{c})$ the non-linear reaction term and ν diffusion coefficient. Reaction term is presented in following subsections.

Equation (1) is complemented with initial conditions

$$\boldsymbol{c}(\boldsymbol{x}, 0) = \boldsymbol{c}_0(\boldsymbol{x}) \qquad \text{on } \Omega$$

Boundary conditions for one dimensional problems, $\Omega = [0, 1]$, are given by

$$\begin{aligned} \mathbf{c}(x, t) &= \mathbf{c}_{ext} \quad \text{on } x = 0 \\ c_x(x, t) &= 0 \quad \text{on } x = 1 \end{aligned} \tag{2}$$

And, for two dimensional problems, $\Omega = [0, 1]\text{x}[0, 1]$, they are written as

$$\begin{aligned} \boldsymbol{c}(\boldsymbol{x}, t) &= \boldsymbol{c}_{ext} \qquad\qquad \text{on } x = 0 \\ \boldsymbol{c}_{\boldsymbol{x}}(\boldsymbol{x}, t) &= 0 \quad \text{on } x = 1 \cup y = 0 \cup y = 1 \end{aligned} \tag{3}$$

where $x = 0$ represents the entrance boundary, while $y = 0$ and $y = 1$ designate the lateral ones and $x = 1$ is the exit boundary.

2.1 Activated Sludge Model No. 1

In 1982 a Task Group on Mathematical Modeling for Design and Operation of Activated Sludge Processes was created in the bossom of the then called International Association on Water Pollution Research Control. This Task Group had the aim of developing a model that could represent the reactions given on the activated sludge processes. Since then, four different models have been released. The first one, named Activated Sludge Model No. 1 (ASM1) was achieved on 1987. It introduced the matrix notation, where both, kinetics and stoichiometry are represented, and it includes modeling of carbon oxidation, nitrification and denitrification. As complexity increases through different release, here the first one is used for illustrating the approach.

The reaction term of the ASM1 model can be written as

$$\boldsymbol{r}(\boldsymbol{c}) = \sum_{j=1}^{8} \nu_{i,j} \rho_j \qquad i = 1, ..., 13. \tag{4}$$

with $\nu_{i,j}$ the stoichiometric coefficients, which express the mass relationships between the components involved in each process, and ρ_j the rate processes. Subindices i and

j are, respectively, the component number and the process number. Sign convention of stoichiometric coefficients is positive for production and negative for consumption (oxygen is expressed as negative oxygen demand).

Processes considered are the following: growth of biomass, separated on aerobic growth of heterotrophs, anoxic growth of heterotrophs and aerobic growth of autotrophs; decay of biomass, also separated on the decay of heterotrophs and autotrophs; ammonification of organic nitrogen and hydrolysis of particulate organics which are entrapped in the biofloc. And components considered on those processes are: soluble inert organic substrate S_I, readily biodegradable substrate S_S, particulate inert organic substrate X_I, particulate readily biodegradable substrate X_S, active heterotrophic biomass X_{BH}, active autotrophic biomass X_{BA}, inert products arising from biomass decay X_P, oxygen S_O, nitrate and nitrite nitrogen S_{NO}, $NH_4^+ + NH_3$ nitrogen S_{NH}, soluble organically bound nitrogen S_{ND}, particulate organic nitrogenX_{ND} and alkalinity S_{ALK}.

2.2 Six–variables model

A simplified six–variables model is also used in this work. This model is a simplification of the ASM1. It represents an aerobic media where only COD removal and nitrification are considered [1]. Reaction term is given by

$$\sum_{j=1,3,4,5} \nu_{i,j}\rho_j \qquad \text{i=2,5,6,8,9 and 10.} \tag{5}$$

It includes four different process, which are the aerobic growth of heterotrophs, $j = 1$ on the ASM1 model; the aerobic growth of autotrophs, $j = 3$; the decay of heterotrophs, $j = 4$; and the decay of autotrophs, $j = 5$. Components involved are $i = 2, 5, 6, 8, 9$ and 10 on the ASM1 notation: S_S, $X_{B,H}$, X_{BA}, S_O, S_{NO} and S_{NH}.

2.3 Oxygen source term

Oxygen equation has, in addition to the corresponding conversion rate of the biochemical model, a source term reflecting oxygen transfer from gas to liquid phases. The change on the oxygen concentration is expressed as [4]

$$K_L a \cdot (S_{O,sat} - S_O) \tag{6}$$

where $K_L a$ is known as Oxygen Transfer Rate (OTR), given by $K_L a = k_1 \cdot \left(1 - e^{k_2 \cdot Q_{air}}\right)$, where k_1 and k_2 are estimated parameters[8].

3 NUMERICAL SOLVER

Spatial part of the problem is approached with the method of weighted residuals, Galerkin formulation. This method leads to symmetric stiffness matrices when applied to problems governed by self-adjoint elliptic or parabolic differential equations. But on convection problems this advantage is not presented. Convection operator is not symmetric, and this may lead to spurious oscillations on the solution, situation that is analyzed later in this section.

High-order time integration of unsteady convection–diffusion–reaction problems is not simple because of the second-order diffusion operator. Here, continuous finite elements are implemented, thus time-stepping schema will only involve first order derivatives [3]. The Runge-Kutta-Fehlberg 4-5 time integration scheme is used [6]. Tolerance imposed has been chosen equal to $0.5\text{x}10^{-4}$.

The outline of the rest of this section follows. First, ASM1 model parameters used in this work are presented. Then, the approach is validated with a simplified six–variables model. One dimensional homogeneous examples are simulated. The influence of oxygen presence in the domain is checked. Section ends with a brief discussion on value of stabilization parameter. Next section present main results of this work, finishing with heterogeneous two dimensional simulations with the whole ASM1 model.

Table 1: Stoichiometric parameters appeared on the ASM1. Source:J. Bolmstedt and G. Olsson, 2002.

Parameter	Value	Units	Definition
Y_H	0.67	g cell COD formed/(g COD oxidized)	yield of growth rate for heterotrophic biomass
Y_A	0.24	g cell COD formed/(g COD oxidized)	yield of growth rate for autotrophic biomass
f_p	0.08		fraction of biomass yielding particulate products
i_{XB}	0.086	g N/g COD in biomass	mass N/mass COD in biomass
i_{XP}	0.06	g N/g COD in endogenous mass	mass N/mass COD in products biomass

3.1 Model Parameters

Model parameters are those of the ASM1 formulation, others which define transport processes and initial and boundary conditions.

Two groups of constants appear on ASM1 model: the stoichiometric and the kinetics parameters. Values used are presented in Tables 1 and 2 respectively. Realistic values are considered, corresponding to a wastewater treatment plant with multi-reactors when its operation temperature is constant and equal to 20°C [1]. Although these values has little relationship with the initial motivation of this work, as a first approach they can be useful to detect the key point of the behavior of this type of convection–diffusion–reaction equations.

On the other hand, parameters of convection-diffusion equation are fixed as $\nu = 10^{-4}$ and $\mathbf{u} = (1, 0)$, corresponding to a situation with low diffusion and a pure horizontal flux.

Table 2: Kinetic parameters appeared on the ASM1. Source:J. Bolmstedt and G. Olsson, 2002.

Parameter	Value	Units	Definition
$\hat{\mu}_H$	6.	h^{-1}	maximum specific growth rate for heterotrophic biomass
K_S	20.	g of COD/m^3	saturation coefficient for heterotrophic biomass
$K_{O,H}$	0.2	g of $0_2/m^3$	oxygen saturation coefficient for heterotrophic biomass
K_{NO}	0.5	g $NO_3 - N/m^3$	nitrate hsc for denitrifying heterotrophs
b_H	0.62	h^{-1}	decay rate for heterotrophic biomass
$\hat{\mu}_A$	0.8	h^{-1}	maximum specific growth rate for heterotrophic biomass
K_{NH}	1.	g of $N_3 - N/m^3$	ammonium saturation coefficient for autotrophic biomass
$K_{O,A}$	0.4	g of $0_2/m^3$	oxygen saturation coefficient for autotrophic biomass
b_A	0.2	h^{-1}	decay rate for autotrophic biomass
η_g	0.8		correction factor for anoxic growth of heterotrophs
k_a	0.08	m^3 / g COD day	ammonification rate
k_h	3.	g slowly biodeg.COD / g cell COD day	max. specific hydrolysis rate
K_X	0.03	g slowly biodeg.COD / g cell COD	hsc for hydrolysis of slowly biodeg. substrate
η_h	0.4		correction factor for anoxic hydrolysis

Dirichlet boundary condition has been fix equal to one for all the unknowns, $\mathbf{c}_{ext} = 1$, and two sets of initial conditions have been defined: $\boldsymbol{c}_0 = 0$ and $\boldsymbol{c}_0 = 1$.

3.2 Approach validation with the six–variables model

In this subsection, results with the six–variables model are obtained and analyzed. A one dimensional domain, $\Omega = [0, 1]$, discretized with 20 equal–size elements, and with initial condition $\boldsymbol{c}_0 = 1$ is solved. No stabilization technique is applied.

Analysis focus in differences due to presence of oxygen. Two limit cases are considered: Entrance of oxygen fixed through the whole domain equal to zero or to a reference value. As it has been previously explained, entrance of oxygen means adding the term on equation

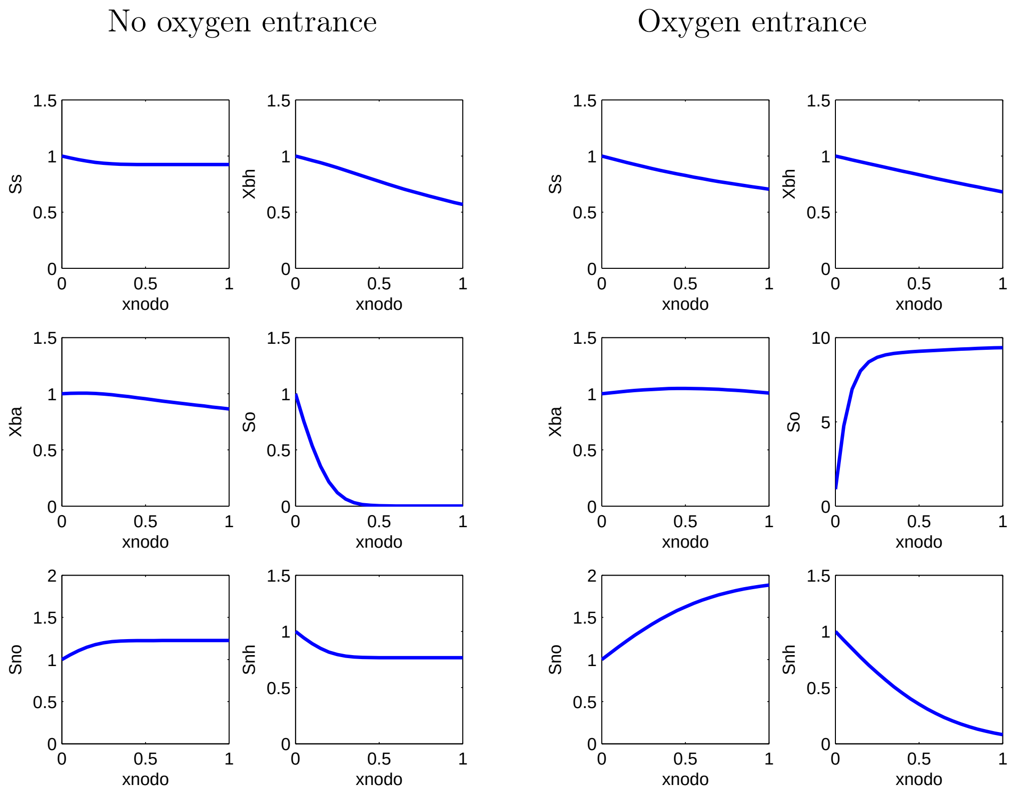


Figure 1: Steady–state results of six–variables model without and with oxygen entrance.

6 on the reaction term in oxygen's equation (S_O). Figure 1) shows concentrations spatial distribution when solution reaches the steady state.

The main differences between both situations are given by S_{NO} and S_{NH}. When presence of oxygen is assured, production of S_{NO} is given while in its absence (on the second half of the domain on the *No oxygen's entrance*'s graphics), there is neither production nor destruction. That occurs so because the process rate on its reaction term goes to zero when absence of S_O is given. A similar situation is given on S_{NH} destruction, as when S_O is not present on the medium, its decreasing is stopped, this time because both processes rates, ρ_1 and ρ_3, become zero. From the biological point of view, as denitrification processes are not considered on this model (only aerobic processes are taken under consideration), destruction of NH_4^+ can not occur without oxygen presence. Therefore nitrate and nitrite can neither be produced.

3.3 Stabilization parameter

Instabilities are found with initial condition equal to zero. Figure 2 show results computed with six variables model and initial condition $\boldsymbol{c}_0 = 0$. Instabilities can be better

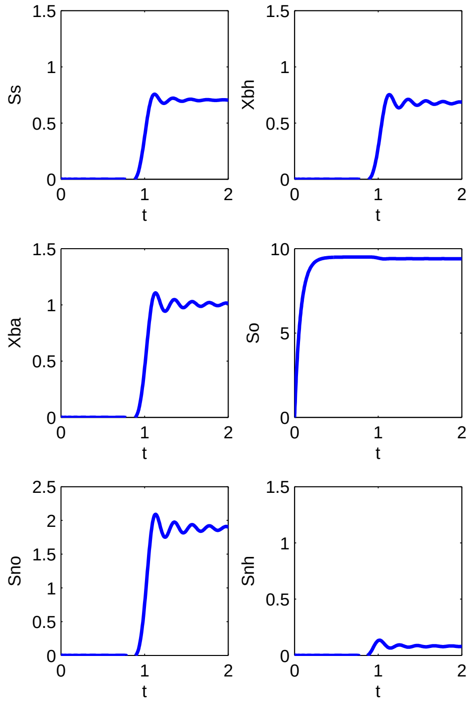


Figure 2: Evolution of six–variables model at $x = 1$ using initial condition $\boldsymbol{c}_0 = 0$.

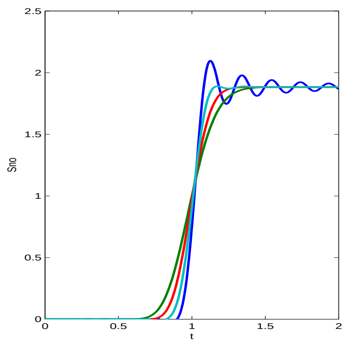


Figure 3: Comparison of S_{NO} evolution at $x = 1$ obtained without stabilization and using $\tau/5$, $\tau/10$ and $\tau/25$.

appreciated on the time-concentration graphic, so on this figure concentration along the time on the exit boundary is presented.

There are different stabilization techniques useful for convection–diffusion and convection–diffusion–linear reaction problems. Examples can be found in [3]. Three of the most used

(Stream Upwind Petrov-Galerkin, Galerkin-Least Squares and Subgrid Scale) end up with the same expression due to the election of linear elements for the spatial discretization. All of them are adequate. However, due to the nonlinear nature of reaction term under consideration, a test to determine the most suitable stabilization parameter is needed.

Figure 3 shows S_{NO} results obtained with $\tau = \frac{h}{2a}\left(\coth(P_e) - \frac{1}{P_e}\right)$ divided by 5, 10 and 25. Solution obtained with $\tau/10$ does not have any perturbation, and its added diffusion is lower than that of $\tau/5$. Therefore that value is considered appropriate to stabilize this type of problems.

4 RESULTS

This section focuses in the solution of the whole ASM1 model in both homogeneous and heterogeneous entrance of oxygen in the domain. Recall that the reference problem under consideration is an uniform horizontal flow, with a source term of oxygen that varies with the vertical coordinate from zero to a reference value.

First, one and two dimensional results for homogeneous problems with and without oxygen entrance are analyzed. After that, first results with heterogenous entrance of oxygen (in the vertical profile) are presented. The suitability of the approach is tested in both problems. Some difficulties arise when discontinuity in oxygen profile appears due to the combination of slow convection and diffusion with respect source term rate. That situation occurs even if a continuous transition in source term rate is imposed.

4.1 Homogeneous examples

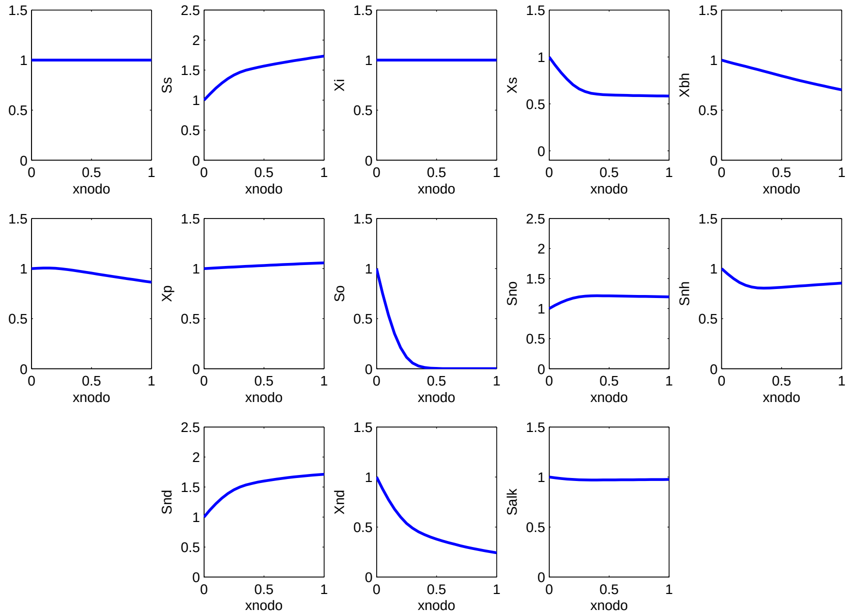
First, one dimensional results obtained with a mesh of 20 equal–size elements are presented and analyzed. After that, it is verified that same results are obtained solving the equivalent two dimensional problem.

Main difference between the six–variables model (Figure 1) and the whole ASM1 (Figure 4), is that with ASM1, S_S is produced instead of destructed. That occurs because hydrolysis of entrapped organics rate is bigger than both of heterotrophs growth. As it may be seen, it continues growing also when oxygen is not present, but with littler velocity due to that one term of this ρ_7 rate is proportional to S_O while the other one is not.

When analyzing both solutions, with and without oxygen, main differences are presented on S_{NO}, S_{NH}, S_S, X_S, S_{ND} and X_{ND} concentrations. Differences on the first two components are the same as on the six–variables model and they have been already described. On X_S and X_{ND}, its destruction is widely increased when oxygen is presented mainly because of its hydrolysis of entrapped organics rates. On the other hand, S_S and S_{ND} production is increased.

From the biological point of view, the small destruction of X_S is because under anoxic conditions (when nitrate is the only terminal electron acceptor) conversion of slowly biodegradable material into readily biodegradable one is lower. Between particulate organic nitrogen and soluble organic one, conversion follows the same patron.

No oxygen entrance



Oxygen entrance

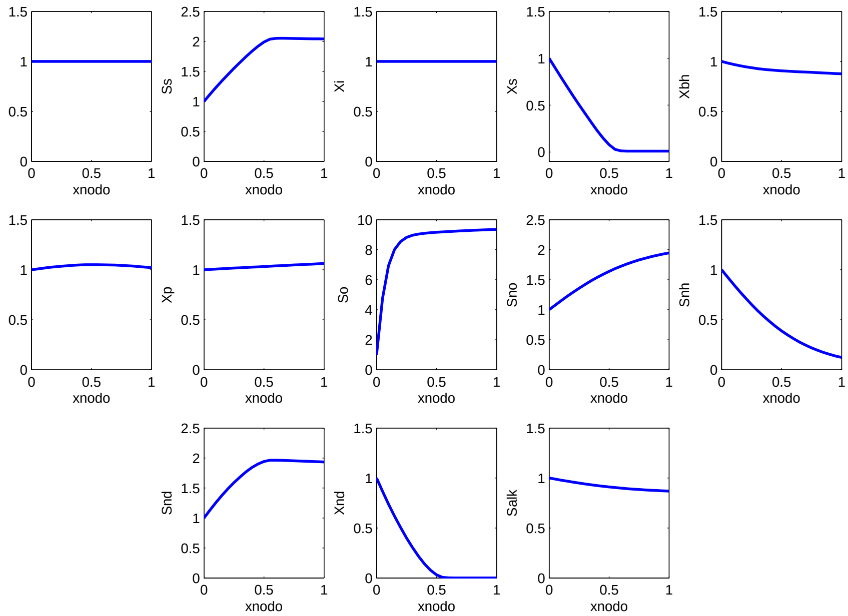


Figure 4: Steady–state results of the whole ASM1 model without and with oxygen entrance. One dimensional simulations.

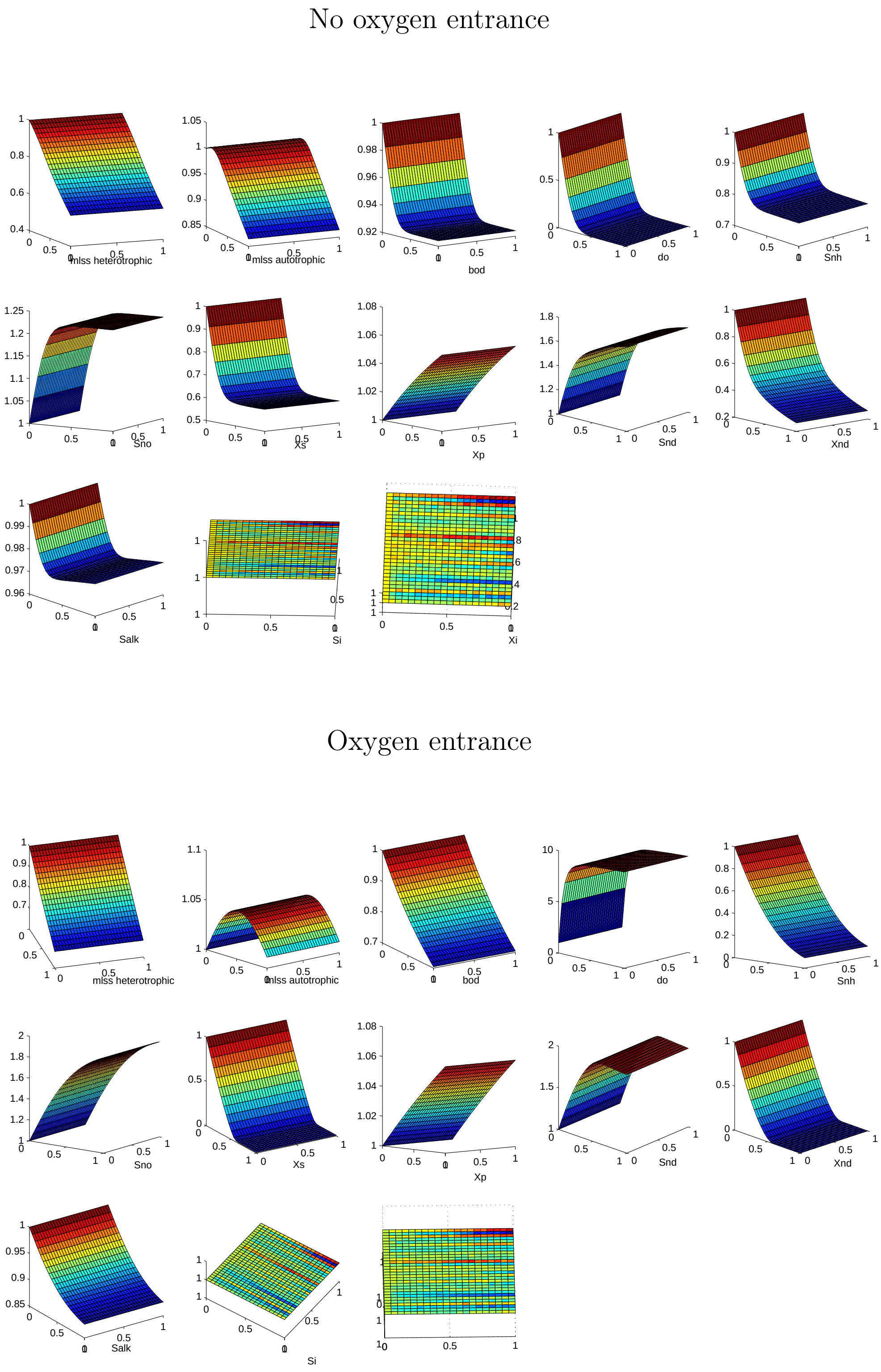


Figure 5: Steady–state results of the whole ASM1 model without and with oxygen entrance. Two dimensional simulations.

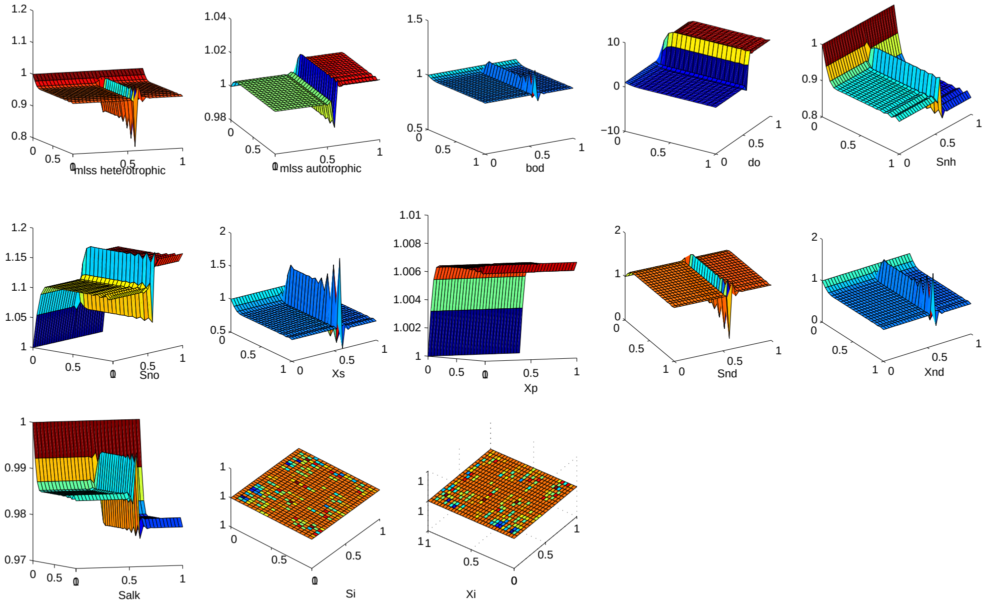


Figure 6: Evolution of concentration on the ASM1 model with oxygen entrance on the upper part of the domain. Discontinuous source term. Final time (dimesionless) 0.1

Two dimensional results on $\Omega = [0,1]\text{x}[0,1]$ have been also computed. A regular mesh of 20x30 quadrangular elements is considered. Both cases, entering oxygen through the whole domain and avoiding its entrance, are considered. Figure 5 shows results, that are, as expected, same of those of one dimensional problem, compare with Figure 4.

4.2 Two dimensional heterogeneous examples

Variation of oxygen entrance in the vertical profile has been imposed in two different ways, with a discontinuous reaction term changing from zero in the lower part of the domain (60%) to the reference value in the upper part; and with a linear continuous transition located between 60 and 80% of height. As the discretization in vertical direction has 30 elements, transition is covered by six elements.

Figure 6 shows results of discontinuous transition of source term, and Figure 7 results of continuous one. Discontinuous approach has been computed up to a final dimensionless time of 0.1, instead of 2 as all the other examples, because of the unbounded spurious oscillations. As a result of the unstability some values become negative. Note that oscillations are caused by discontinuity of oxygen. The flux has only entered 10% of domain length.

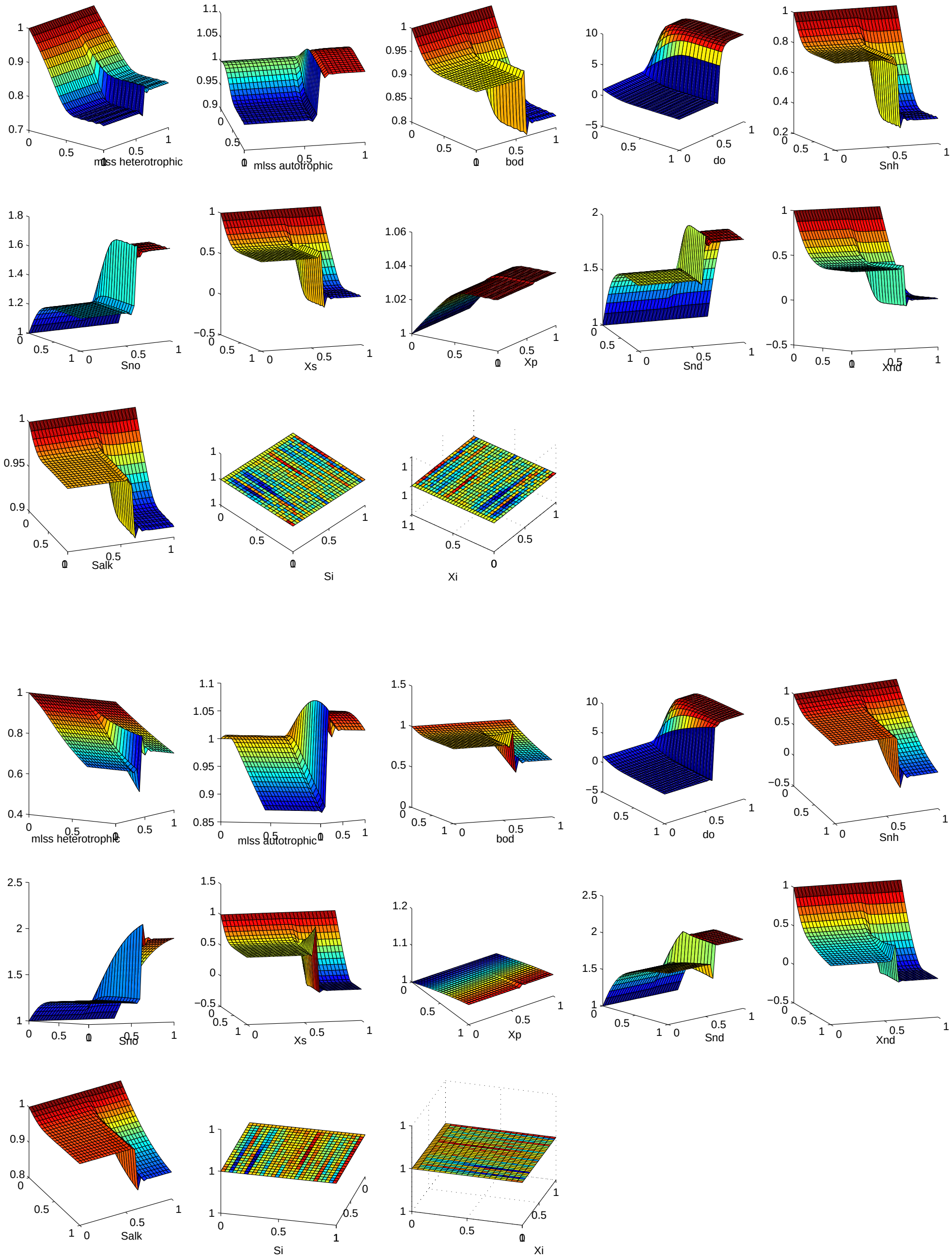


Figure 7: Evolution of concentration on the ASM1 model with oxygen entrance on the upper part of the domain. Continuous source term. Final time (dimesionless) 0.5 (up) and 2 (bottom).

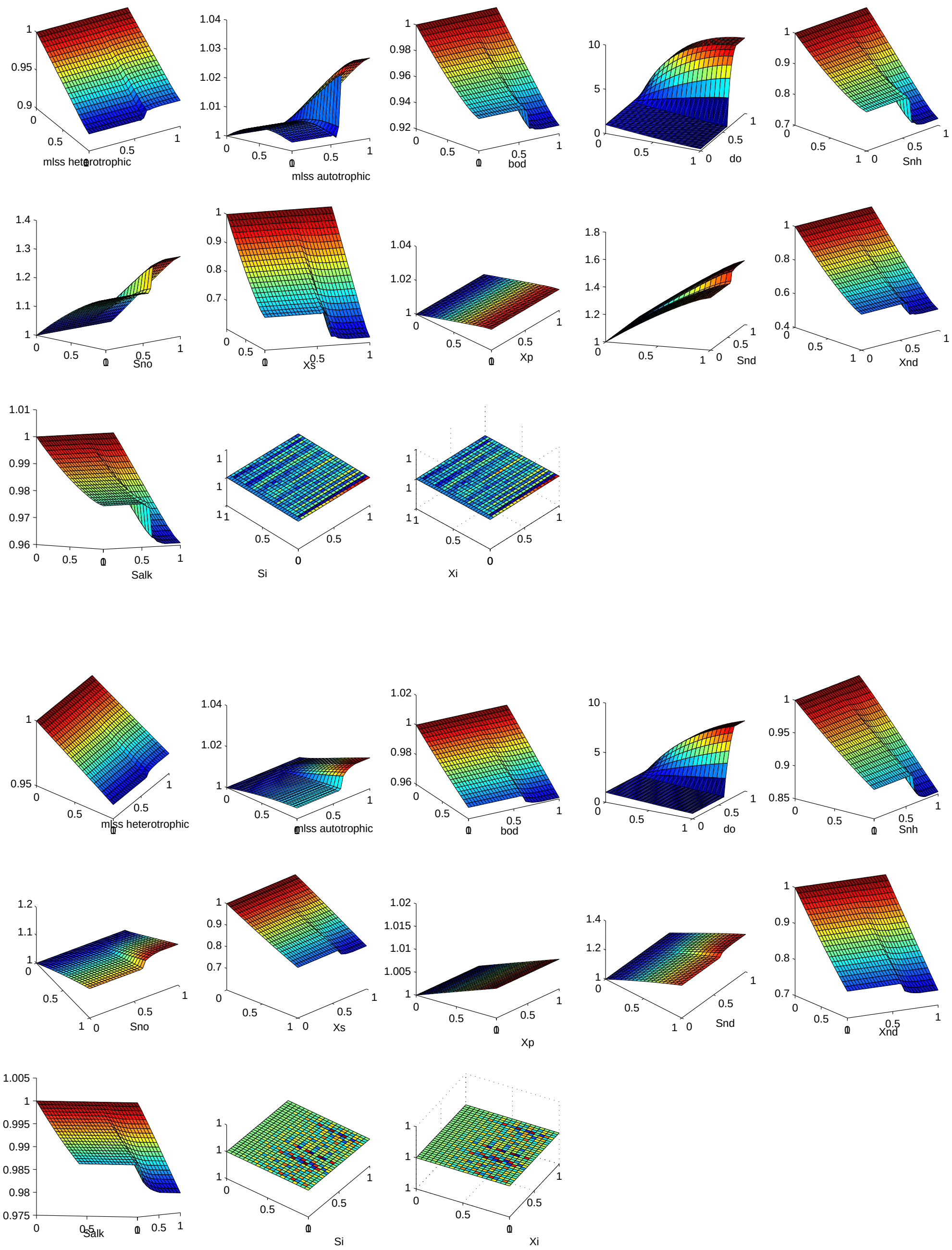


Figure 8: Evolution of concentration on the ASM1 model with oxygen entrance on the upper part of the domain. Continuous source term. Dimesionless velocity 5 (up) and 10 (bottom).

Results with a continuous transition of oxygen entrance are better simulated. Figure 7 show distributions for final dimensionless time equal to 0.5 and 2. Steady-state is found (under constant loading) just after wave propagation throughout the domain (with dimensionless velocity equal to one). Note that spurious oscillations still appears around sharp variation of oxygen profile in vertical direction. They increases as the problem evolves, but they remain bounded and do not disturb solution of the problem except for the local oscillation itself.

As it has been shown, oscillation is directly related to oxygen discontinuity. Moreover, oxygen discontinuity can be directly related to different relative velocities between oxygen source/reaction term and convective transport. Results increasing horizontal velocity by a factor 5 and 10, which are presented in Figure 8, confirm that relationship.

5 CONCLUSIONS

A stabilized finite element formulation combined with a high order time-integration adaptative scheme has been applied to two dimensional transport – biochemical reaction problems including a dissolved oxygen source term with an heterogeneous distribution. The approach has been applied considering the ASM1 model and a simplified geometry and velocity flow field. Extension to other biochemical models and general geometries and velocity fields should be straightforward.

Although the approach has been applied successfully, further developments are needed to manage discontinuities of the unknowns when produced by source terms (as the oxygen entrance simulated here) and slow velocity fields are present. Standard stabilization useful for convection dominate problems is not able to reduce spurious oscillations if discontinuities are parallel to flux. Discontinuities appear only with reduced flow velocities with respect reaction velocity of the source term.

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