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Application of a model-based method for hydrodynamic processes in constructed wetland for the management of livestock wastewater based on finite elements method

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ABSTRACT

In this article, a mechanistic process-based model is developed, for accurate predictions of pig farms wastewater behavior in free water constructed wetlands. Twenty-six variables were considered in order to simulate the simultaneous hydraulic, physical, biochemical and physico-chemical characteristics of different processes that are happening in this system. The proposed model was developed by optimization of the advection-diffusion-reaction equations. For that, Stokes equations and the Anaerobic Digestion Model No. 1 were implemented. The mathematical analysis of the model involves the use of a numerical model, the finite element method, and flowchart-based strategy planning. Numerical simulation in a two-dimensional model using open access software (FreeFem++) are presented to demonstrate the dynamic behavior of the proposed prototype.

Keywords: Free water constructed wetlands; Anaerobic Digestion Model No. 1; Advection-diffusion-reaction equation; Stokes; Anaerobic process

1. Introduction

Today, around 80% of all wastewater is discharged into the world's waterways due to poor water planning and extensive urbanization and industrialization [1,2]. Together with the increase in production and concentration of intensive livestock operations, wastewater treatment (WWT) mismanagements have raised the risk of contamination to the environment [3].

Increasingly strict environmental regulations have created the need to find solutions, which combine low-cost facilities and resource efficiency in WWT [4]. In this context, constructed wetlands (CWs) are now more widely applied than other technology as a WWT alternative, in developing countries [5–7]. However, the performance of CWs is still too difficult to predict, due to the diversity and simultaneousness of the physical, chemical and biological processes involved, some of which are yet to be understood [8]. During the last decade, several mathematical models for the description of the behavior of CWs have been published [9]. Nowadays, most efforts in this specific field are centered on the development of mechanistic or process-based models (PBMs), which not only predict effluent pollutant concentrations but can also shed light on the treatment processes involved. For this reason, these kinds of models are gaining prevalence over simple black box [10] or first-order decay ones [11]. The vast majority of PBMs has been developed for simulating subsurface flow WWT systems, with CWM1 [12], CW2D [13] and BIO-PORE [14] some of the most robust and widely accepted models. However, these types of models are less abundant for the simulation of free water surface (FWS) systems, and

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those that are available often include a limited number of components and interactions [15–17].

In this paper, an original model is presented to describe the process of simultaneous physical, biochemical, hydraulic and physico-chemical characteristics in FWS CWs. The proposed model was developed from the basic advection-diffusion-reaction (ADR) equations [18], and the Anaerobic Digestion Model No. 1 (ADM1) proposed by the International Water Association (IWA) [19]. A general finite element method (FEM) [20], based on a suitable stabilization of the Galerkin formulation, was used for the calculation.

The main goal of this paper is the introduction of free software, with a high-level programming language, for CWs simulation in anaerobic processes. The methodology enables the combination of several mathematical modellings in the form of a first order conservation law system, with inclusion of different kinetic models.

2. Model development

2.1. General formulation

The ADR equation is used to represent the processes involved in CWs. Transport phenomena are described with the Stokes equations, considering an incompressible Newtonian fluid in steady state, and the reaction system, which takes place in the anaerobic domain in CWs, is derived from basic structure of the ADM1, which includes biochemical and physico-chemical reactions. The numerical method used, FEM, plays a significant role in finding the numerical solutions for two classes of ADR. The ADR equation, in a finite domain, was studied taking a two-dimensional nonlinear problem with decay and source terms into account. The boundary value problem (BVP) admitted in this work, was the combination of the Dirichlet and Neumann boundary conditions. The BVP was defined by fully restraining the top, bottom and the left side. The general conditions of this study and the related finite element discretization with boundary conditions are presented in Fig. 2.

The transient transport equation for a scalar quantity $\varphi(x,y,z,t)$ undergoing constant ADR is given by Eq. (1):

$$\frac{\partial \phi}{\partial t} = D\Delta\phi + u\nabla\phi + f \tag{1}$$

where φ is the field variable content in a unit area of the system, t is the time of exposure, D is the diffusion coefficient $D = D_x = D_y = D_z$ = constant, the operator 'Δ' is defined by $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$, and the operator '$\nabla$' is defined by $\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$, the parameters $u(u_1,u_2,u_3)$ represent the velocity coefficients obtained by the Stoke equation (Eq. (2)), and the function f describes the anaerobic processes which include the growth and decay of biomass and substrates removal.

2.1.1. Stokes problem

The incompressible Stokes equation describes the velocity $\vec{u}$ in a bounded or unbounded domain of R^n, n = 2, 3 [21,22]. In this case (R^2), this equation, for steady flow, is given by:

To find $\vec{u} = (u_1, u_2)$ and p such that:

$$\begin{aligned} -v\Delta\vec{u} + \nabla p &= \vec{f} \quad \text{in } \Omega \\ \nabla\vec{u} &= 0 \quad \text{in } \Omega \\ \vec{u} &= g \quad \text{on } \partial\Omega \end{aligned} \tag{2}$$

where Ω is a polygonal domain in R^2, $\vec{u} = (u_1, u_2)$ represents the velocity and p is the pressure, v is the viscosity coefficient, and $\vec{f}$ is an external force affecting the system. The Dirichlet boundary condition is Γ_D and the Neumann boundary condition Γ_N, such that $\partial\Omega = \Gamma_D \cup \Gamma_N$.

2.1.2. Anaerobic processes

The ADM1 is based on sewage sludge anaerobic digestion and gives a unified representation of disintegration, hydrolysis, acidogenesis, acetogenesis and methanogenesis [23]. This model, developed by the IWA task group, is a mathematical model mainly describing the biochemical processes (Fig. 1) involved in anaerobic digestion [19].

The model, which has been categorized into two biochemical and physico-chemical frameworks, contains a total of 30 dynamic state variables from substrates and cells.

2.1.2.1. First biochemical processes

ADM1 employs a set of 24 differential rate equations to describe the biochemical processes involved in anaerobic digestion. The disintegration, hydrolysis and bacterial decay steps are represented by first order kinetics, while all the other steps are represented by Monod-type kinetics [24] (Fig. 1). The equation, which was proposed by Monod in 1949, for describing microbial growth [25], is as follows:

$$\rho_j = \mu_{\max_i} \frac{S_i}{K_{S_i} + S_i} \times I_{\text{pH}} \tag{3}$$

where ρ_j (d^{-1}) is the specific growth rate, $\mu_{\max_i}$ (d^{-1}) is the maximum specific growth rate, S_i (kg m^{-3}) is the substrate concentration, K_{S_i} (kg m^{-3}) is the substrate saturation constant (i.e., substrate concentration at half $\mu_{\max}$) and I_{pH} is the inhibition function, which considers growth rate inhibition due to pH (Eq. (5)). The kinetic rate of each process is represented by ρ_j. The parameter values can be found in the works of Batstone et al. [19] and Zhang et al. [24].

To describe the consumption of substrate and microbial growth, the following expression was proposed

$$\frac{dS_i}{dt} = -\rho_j \frac{X_i}{Y_i}; \quad \frac{dX_i}{dt} = \rho_j X_{i\,\text{pH}} - K_d X_i \tag{4}$$

where $\frac{dS_i}{dt}$ (kg m^{-3} d^{-1}) is the change in substrate concentration, X_i is the biomass concentration (kgCOD m^{-3}), Y_1 is the substrate yield coefficient, $\frac{dX_i}{dt}$ (kgCOD m^{-3} d^{-1}) is the change in cell concentration over time and K_d (d^{-1}) is the cell death rate.

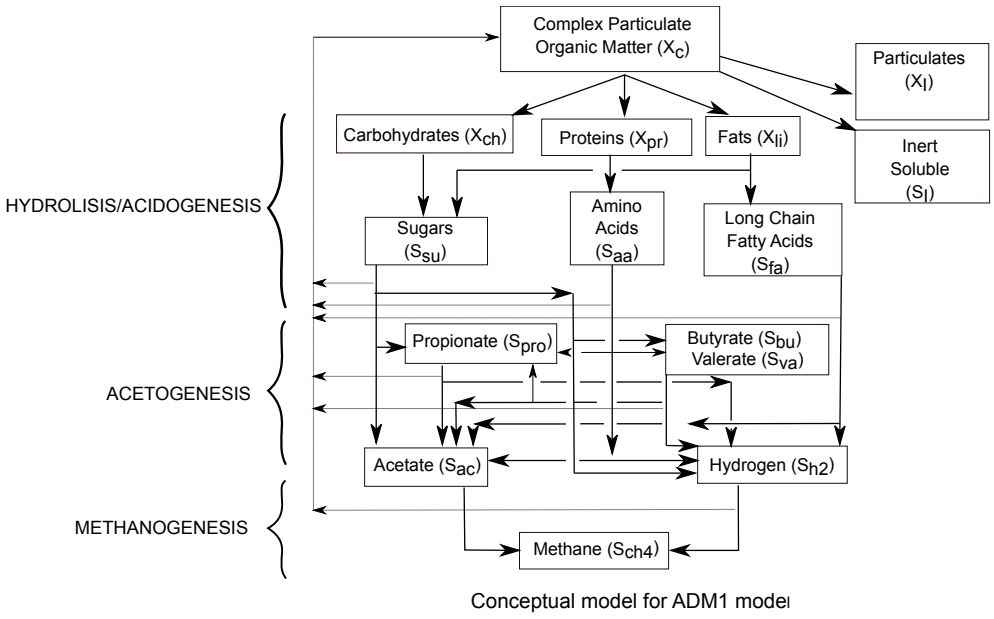

Fig. 1. Anaerobic processes flow chart, according to ADM1.

The growth rate inhibition due to pH is given by:

$$I_{\mathrm{pH}} = \exp\left(-3\left(\frac{\mathrm{pH}-\mathrm{pH}_{\mathrm{LL}}}{\mathrm{pH}_{\mathrm{UL}}-\mathrm{pH}_{\mathrm{LL}}}\right)\right) \tag{5}$$

The given values for the upper and lower pH are: $\mathrm{pH}_{\mathrm{UL}}$ = 7.35 and $\mathrm{pH}_{\mathrm{LL}}$ = 4.77, according to experimental data [19].

2.1.2.2. Second physico-chemical processes

The original ADM1 incorporated six acid–base reactions which describe the acid/base equilibria of acetic acid/acetate, propionic acid/propionate, butyric acid/butyrate, valeric acid/valerate, dissolved carbon dioxide/bicarbonate and ammonium/ammonia. The corresponding equation is:

$$z+\left[\mathrm{NH}_4^+\right]+\left[\mathrm{H}^+\right]-\left[\mathrm{HCO}_3^-\right]-\frac{\left[\mathrm{Ace}\right]}{64}-\frac{\left[\mathrm{Prop}\right]}{112}-\frac{\left[\mathrm{But}\right]}{160}-\frac{\left[\mathrm{Val}\right]}{208}-\left[\mathrm{OH}^-\right]=0 \tag{6}$$

where the different terms (kg m^{-3}) of the equation are:

$$\left[\mathrm{HCO}_3^-\right]=\frac{\left[\mathrm{CO}_2\right]K_C}{\left[\mathrm{H}^+\right]};\quad \left[\mathrm{NH}_4^+\right]=\frac{\left[\mathrm{NH}_3\right]\left[\mathrm{H}^+\right]}{K_N};$$
$$\left[\mathrm{AGV}^-\right]=\frac{\left[\mathrm{AGV}\right]K_{\mathrm{AGV}}}{\left(\left[\mathrm{H}^+\right]+K_{\mathrm{AGV}}\right)M_{\mathrm{AGV}}} \tag{7}$$

where K_C, K_N, K_{AGV} are the acid–base reactions equilibrium coefficients.

2.1.3. ADR for dynamic state variables

Dynamic state variables are those calculated at a specified time (t) by solution of the set of differential equations as defined by the ADM1 process rates [19].

The ADR equation for substrate is given by:

$$\begin{cases} D\Delta S_i + u\nabla S_i + \rho_j \dfrac{X_i}{Y_i} = \dfrac{\partial S_i}{\partial t} & \text{in } \Omega \\ S_i = S_{i_0} & \text{in } \Gamma_D \text{; BC} \\ \dfrac{\partial S_i}{\partial n} = 0 & \text{in } \Gamma_N \text{; BC} \end{cases} \tag{8}$$

where S_i is related to each one of cells included into the 24 state variables described by ADM1.

The ADR equation for cells is given by:

$$\begin{cases} D\Delta X_i + u\nabla X_i - \left(\rho_j X_{i\,\mathrm{pH}} - K_d X_i\right) = \dfrac{\partial X_i}{\partial t} & \text{in } \Omega \\ X_i = X_{i_0} & \text{in } \Gamma_D \text{; BC} \\ \dfrac{\partial X_i}{\partial n} = 0 & \text{in } \Gamma_N \text{; BC} \end{cases} \tag{9}$$

where X_i is related to each one of substrates included in the 24 state variables described by ADM1

2.2. Variational form of the conservative equation

The transient and steady-state problems given by Eqs. (8) and (9), respectively, can be solved by the FEM. In this technique, termed the generalized integral transform technique (GITT), the unknown function is represented in terms of an eigen function series expansion. Basically, the GITT has the following steps:

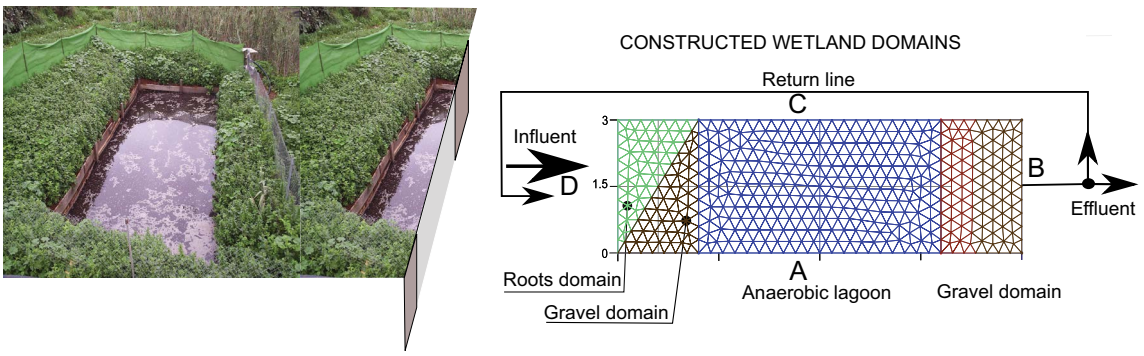

Fig. 2. Discretization of the domain triangle = 1,170; vertex = 643.

(i) Discretization of the domain (Fig. 2).
- Choose the appropriate domain and sub-domain

(ii) Formulation of the partial differential equations for the equivalent variational problem
- Develop the integral
- Transform the partial differential equation into a system of ordinary differential or algebraic equations
- Solve the ordinary differential or algebraic system. Use the inverse transform to obtain the unknown function

The variational form of the boundary-value problem is stated in terms of the following functions spaces.
(i) Velocity: the weak Galerkin method developed in 2.1.1 for the Stokes equations naturally has the form [26]: to find u: $\Omega \subset R^2 \to R$ such that

$$\begin{cases} v\int_\Omega \nabla\vec{u}\nabla\vec{v} - \int_\Omega \operatorname{div}\vec{v}p = \int_\Omega \vec{f}\vec{v} & \text{for } \vec{v}\in\left[\mathrm{H}_0^1(\Omega)\right]^2, \\ \int_\Omega (\operatorname{div}\vec{u})q = 0 & \text{for } q\in L^2(\Omega)\text{IC} \\ \int_\Omega p = 0 & \text{solubility condition} \\ \vec{u}(x) = \vec{h}_D(x) & \text{for } x\in\Gamma_D\subset\partial\Omega, \text{ BC} \\ \vec{u}(x)\vec{\eta} = \vec{h}_N(x) & \text{for } x\in\Gamma_N\subset\partial\Omega, \text{ BC} \end{cases} \tag{10}$$

where $\vec{v}$, q are smooth functions.

(ii) Cells
To find X_i: $\Omega \subset R^2 \to R$ such that

$$\begin{cases} \mu\int_\Omega \frac{\partial X_i}{\partial t}W_i + D\int_\Omega \nabla X_i\nabla W_i d\Omega + \int_\Omega \vec{u}\nabla X_i\nabla W_i d\Omega = \int_\Omega \left(\rho_j X_{i\,\mathrm{pH}} - K_d X_i\right)W_i d\Omega & \text{for } X_i\in\left[\mathrm{H}_0^1(\Omega)\right]^2 \\ X_i(x,y,t) = g_D(x,y) & \text{for } x,y\in\Gamma_D\subset\partial\Omega, t>0 \\ \nabla X_i(x,y,t)\eta(x,y) = g_N(x,y) & \text{for } x,y\in\Gamma_N\subset\partial\Omega, t>0 \\ X_i(0,x,y) = X_{i_0}(x,y) & \text{for } x,y\subset\Omega \end{cases} \tag{11}$$

(iii) Substrate
To find S_i: $\Omega \subset R^2 \to R$ such that

$$\begin{cases} \int_\Omega \frac{\partial S_i}{\partial t}W_i + D\int_\Omega \nabla S_i\nabla W_i + \int_\Omega u\nabla S_i W_i = \int_\Omega \left(\rho_j X_i\right)W_i & \text{for } S_i\in\left[\mathrm{H}_0^1(\Omega)\right]^2 \\ S_i(x,y,t) = g_D(x,y) & \text{for } x,y\in\Gamma_D\subset\partial\Omega, t>0 \\ \nabla S_i(x,y,t)\eta(x,y) = g_N(x,y) & \text{for } x,y\in\Gamma_N\subset\partial\Omega, t>0 \\ S_i(0,x,y) = S_{i_0}(x,y) & \text{for } x,y\subset\Omega \end{cases} \tag{12}$$

where W_i is the smooth function.

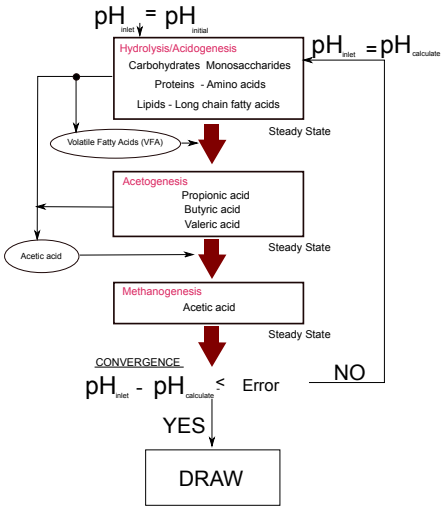

Fig. 3. Flowchart of the strategy used for the calculation.

2.3. Calculation

An algorithm, combined with the FEM is proposed in this study. Fig. 3 shows the strategy used for the calculation. The methodology is as follows: the biochemical processes of the anaerobic digestion are divided into three overall levels.

(i) Steady state of each one of the biochemical steps of a level is attained before starting with the following.
(ii) Finally, the resulting pH of the physico-chemical process is compared with the initial pH, and the difference gives the convergence to the final solution.

FreeFem++ was used to implement the algorithm for the calculation. It is a partial differential equation solver with its own high-level language [27]. FreeFem scripts can solve multiphysics nonlinear systems in 2D and 3D. Space discretization was carried out using the Gmsh, a free finite element mesh generator [28].

3. Results and discussion

The resulting discretization of the problem has included 1,170 triangles and 643 vertices, organized into four domains (Fig. 2). The boundary conditions taken into account were the following: continuous flux, load and discharge in D and B, and part of the effluent in D is returned to influent. Along the top and bottom boundaries (sections A and B), we imposed a non-slip boundary condition for the Stokes equations and non-penetrable boundary condition for the ADR equation. We considered a continuous flux with the value shown in Table 1.

Several simulations with different rates of substrate and fluxes were carried out. We considered that specific growth rate (ρ_j) depends on the growth medium composition, substrate concentration and the acid/base equilibria.

As can be seen, the results agree with the theory, that is, we observe at least a first convergence rate for all variables

Qualitatively, the ADR equation agrees with the flow. The concerned biological species tend to follow the flow according to the velocity field of Stokes equation because of the boundary conditions set. In this case, fluid is transported

Table 1
Boundary conditions

Concentration		A	B	C	D
Substrates (kg m^{-3})	$X_{i\,\mathrm{ent}}$	0	0	0	100
Cells (kg m^{-3})	$S_{i\,\mathrm{ent}}$	0	0	0	10
Flow (m^3 d^{-1})	Q	0	9	0	9

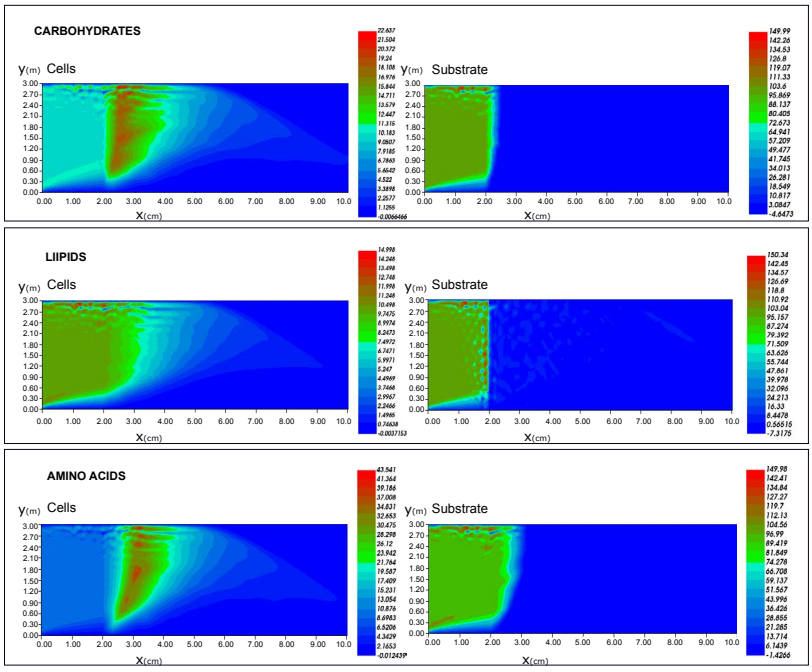

Fig. 4. Concentrations (kg m^{-3}) and distributions of biochemical steps for acidogenesis.

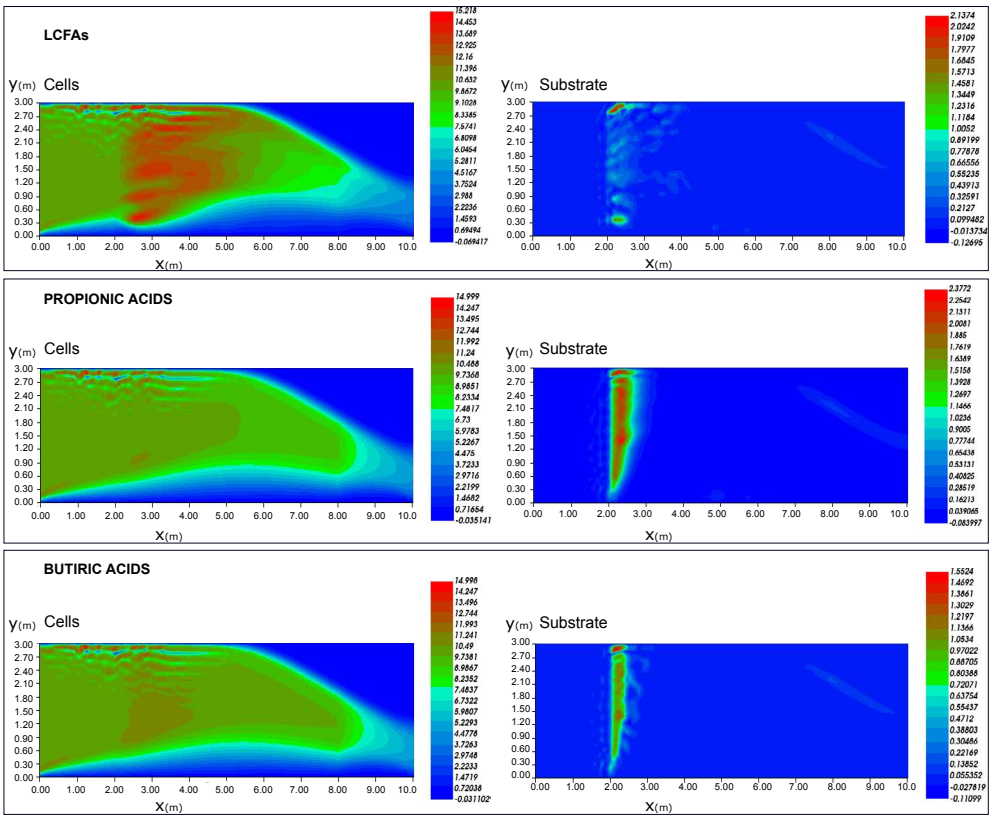

Fig. 5. Concentrations (kg m^{-3}) and distributions of biochemical steps for acetogenesis.

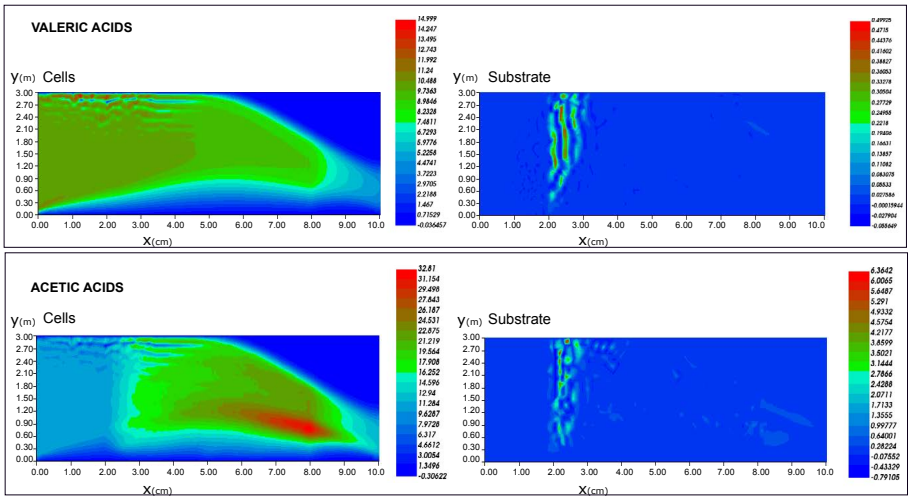

Fig. 6. Concentrations (kg m^{-3}) and distributions of biochemical steps for acetogenesis and methanogenesis.

toward the opening in the right boundary following the Stokes velocity profile and with little diffusion happening, which agrees with the parameters we set for the transport equation.

The boundary and initial conditions in this example are represented in Table 1.

The diffusion coefficient considered is $8.64e^{-3}$(m^2 d^{-1}).

The concentrations and distributions of solutions for the different biochemical steps in steady state are shown in Figs. (4)–(6). Cells are represented on the left and contaminants on the right.

If we compare the different biochemical steps, we see:

- First, with respect to concentrations
- For the example of acidogenesis (Fig. 4), such that processes occur in a simultaneous way, domain group of cells is located in the amino acids step, nevertheless, in the lipids we find cells with a lower concentration.

- Second, with respect to distribution
- Comparing acidogenesis to acetogenesis (Figs. 4 and 5), we can see that distribution of cells depends on the product of the previous process, so microbial growth tends to occur near the source.

4. Conclusion

In this work, an original model is presented to describe the different processes that take place inside CWs. A free fluid in a system was considered, which operates in the same way as a plug-flow reactor, whose hydraulic, physical, biological and physico-chemical characteristics depend on time and position. In the latter, we considered growth-limiting functions which depended on factors such as growth medium composition, substrate concentration and pH. The ADR equation, including fluid flow and transport mathematical expressions, based on the Stokes equations in steady state, was used throughout the whole process. The ADM1 model was used for microbial kinetics. We obtained 26 variables to be solved.

The FEM was used to describe mathematical modelling approaches, allowing for robust and efficient numerical simulation of the processes. FreeFem++ and Gmsh were the tools used for the calculation.

An analysis of the model was performed, and it shows how cell behavior differed depending on the biochemical step involved.

Finally, a realistic example, with a set boundary conditions values, is shown. In it, the flow and concentration of species and substrates is performed simultaneously.

The potential extensions of this work include a development of parallel non-overlapping domain decomposition methods and algorithms.

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